# Research at the Energy Frontier at Southern Methodist University 

## Final report

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## 1. Overview

This grant covered an umbrella program of research in high-energy particle physics at Southern Methodist University during the period 2004-2013. The experimental program evolved during that time. At its early stages it included research on the CLEO experiment at CESR (Coan, Stroynowski, Ye), D0 experiment at Tevatron (Kehoe), preparation for the BTEV experiment at Fermilab (Coan) and construction and commissioning of the Liquid Argon Calorimeter for the ATLAS experiment at LHC (Stroynowski, Ye). In the last three years the program concentrated on the ATLAS experiment at LHC (Kehoe, Sekula, Stroynowski, Ye), D0 experiment at Tevatron (Kehoe) and NOvA experiment at Fermilab (Coan). Professor Sekula had a short-term independent grant for which he is submitting a separate report. The theoretical physics program included work on non-perturbative methods in the light cone representation (McCartor (deceased)), lattice calculations (Hornbostel), and determination of parton distribution functions (Olness). A summary of the accomplishments emphasizing results from the past three years is provided separately for each of the tasks.

## 2. ATLAS.

The SMU group has been among the founding members of the US ATLAS program. Stroynowski co-authored the 1994 LOI submission. Ye joined in 1997, Kehoe in 2004 and Sekula in 2009. During the detector construction phase SMU was responsible for the optical data links and parts of the front-end electronics of the Liquid Argon Calorimeter. Stroynowski and Ye are part of the ATLAS Liquid Argon Collaboration. Maintenance of the links and the handling of their operational problems remains their primary responsibility. Stroynowski has been the US-ATLAS Level-2 manager for the Liquid Argon Calorimeter system during the detector design, construction, installation and commissioning. He relinquished his responsibilities in 2010 to devote his time to data analysis. Ye lead the electronics group at SMU. His R\&D program resulted in the world's fastest ASIC serializer chips, exceeding 5 Gbps , designed for HEP applications. His program is on track towards a goal of 200 Gbps per Front-End Board planned for the ATLAS detector upgrade. In 2011 Ye was appointed as the Level-2 manager for the US-ATLAS LAr upgrade program. He also coordinates US efforts with our European colleagues. In addition, Ye has been elected as the ATLAS convener in the joint ATLAS-CMS optoelectronics working group. During the commissioning and operations phase, our SMU group's responsibilities expanded to the areas of the Trigger and Data Acquisition and to the detector operations and Data Quality. Kehoe established the initial TDAQ organization for the Liquid Argon calorimeter and its connection to the overall ATLAS system. He was appointed a convener of the Liquid Argon Calorimeter TDAQ/Data Quality performance group for 2005-2008. His primary focus has been physics analysis, and has been appointed co-convenor of the H $\rightarrow$ WW Theory study group. Kehoe and Sekula are now members of the ATLAS TDAQ Collaboration. Sekula worked on trigger performance for the 2011-2012 run and explored the calorimeter trigger changes required for the Phase I detector upgrade. He has been appointed a co-convener of the ATLAS supersymmetric Higgs study group. The overall ATLAS effort at SMU was shared among the maintenance and operation tasks of the experiment, a significant involvement in data analyses and R\&D towards the ATLAS upgrade.

### 2.1 Recent Research Activities and Accomplishments

Even though the individual faculty members have well-defined areas of responsibility, there is a significant internal collaboration and sharing of effort to fulfill ATLAS requirements towards the operation of the experiment, shifts and in the sharing of expertise in data analyses. During the last three years Sekula supervised postdoc Aidan Randle-Conde and graduate student Tingting Cao. Stroynowski supervised postdocs David Joffe, Julia Hoffman and some of the work of Ana Firan and graduate students Rozmin Daya, Renat Ishmukhametov and Ryan Rios and shared with Ye the supervision of Andy Liu. Ye supervised postdocs Hulin Wang, shared the supervision of postdoc Ana Firan and led the electronics group of Andy Liu, Annie Xiang, Datao Gong and Kent Liu. Finally, Kehoe supervised, on the ATLAS experiment, postdocs Haleh Hadavand, Peter Renkel, software engineer Sami

Kama, and graduate students Yuri Ilchenko, Pavel Zarzhitski, Azeddine Kasmi and Kamile Dindar. The group size was largest in 2010 and has shrunk in the following year due to graduations and departures. In 2012 the base program supported 3 postdocs and 1 graduate student. Kama, Liu, Xiang and Gong were supported by the ATLAS Project and by the Versatile Link Project funds. The group shared the experiment's operations tasks that included shifts, software development and improvements and creation of various monitoring displays for the ATLAS Control Room.

ATLAS has been a very productive experiment. At the time of this writing there have been over 250 papers published in the refereed journals and about 490 conference submissions. The discovery of the Higgs boson is considered to be the main accomplishment of the last three years. In addition, however, no phenomena expected from physics beyond the Standard Model have been observed in the energy range below 1 TeV . Since the beginning of data taking SMU group has been very active in several data analyses described in the following sections. There have been significant contributions to 16 ATLAS publications, 26 conference papers and a large number of internal ATLAS support notes. These, together with work on the electronics developments ( 6 papers) are described in the following sections. Additional notes and presentations not discussed in the following sections are listed in Refs. [J1, M1-M10]. Only papers that have been published and had significant SMU contribution are appended to this report.

In the following we describe work done under individual supervisions. The collaborative efforts are cross-referenced with names attached to the titles.

### 2.2. Stroynowski (with Joffe, Hoffman, Firan, Daya, Ishmukhametov, Rios and Ye)

After 14 years of service Stroynowski relinquished in 2010 his responsibilities as the US-ATLAS Level-2 manager for the Liquid Argon Calorimeter system to devote more time to data analysis. He spent his 2010/2011 sabbatical leave at CERN. He applied his knowledge of the calorimeter to physics analyses with signatures of electrons, photons and highly ionizing particles. Early work included: the development of the software for the reconstruction of gamma conversions; measurements of single- and double-photon spectra; improvements of the electron identification near the edges of the detector; improvement of the track-cluster matching using a Gaussian Sum Filter; and to the searches for the Higgs boson signal in two photon and four lepton final states and searches for the high mass dilepton resonances and other signatures of physics beyond the Standard Model. The focus of recent work has been on the Higgs search in the 4 -lepton final state ( $4 \mathrm{e}, 2 \mathrm{mu} 2 \mathrm{e}$ and 4 mu ). This work resulted in a large number of internal ATLAS notes and significant contributions to many conference and journal papers. The calorimetry signals expertise was applied also to a number of analyses with large groups of collaborators as described later. Finally, Stroynowski served on an editorial board for the 2011 ATLAS paper on excited lepton searches and was an internal reviewer of several general ATLAS and specialized Liquid Argon calorimeter papers,
conference notes and posters and participated in US ATLAS reviews of computing and LAr Calorimeter upgrade.

## Detector Operations and Service Work

a) Optical links (with Ye and Liu)

The maintenance of the LAr optical data links remains a major hardware responsibility of the SMU group as part of US ATLAS M\&O program. Shortly after the closure of the detector in 2009 we observed failures of the links that were identified as due to the catastrophic failures of the VCSELs on the transmitter (OTx) units. Extensive studies concluded that the failures were due to humidity penetrating broken packaging of the VCSELs that had been damaged during OTx assembly. The spectrum width of a VCSEL was found to be a good indicator of its lifetime. About 70 Front End Boards that exhibited narrow optical spectrum (i.e. had OTx suspected to be affected by humidity) were replaced with spares during the December 2010 shutdown and no new OTx failures were observed since then.
b) Detector operations (with Hoffman, Rios, Ishmukhametov, Daya and Firan)

Hardware-related work included development of the calorimeter control panels for the ATLAS Control Room and calibration and cross-talk measurement of the LAr calorimeter readout channels. Rios developed a series of control and monitoring panels for the high- and low-voltage systems and an overall shifter panel. These had to be periodically updated for each new release of the TDAQ software. Rios was an on-line expert for the 2009-2011 run periods and developed a number of automatic recovery procedures for several types of detector failures. These increased the data taking efficiency to close to 99\%. For the 2011-2012 runs Rios and Hoffman became Shift Leaders for the 14 person ATLAS shift crews. Firan took a substantial number of calorimeter data quality monitoring shifts.
c) Software developments (with Joffe, Hoffman, Daya and Ishmukhametov)

1. Ishmukhametov used the LAr readout calibration system to measure the cross talk between the 173,000 individual readout channels. The procedure was developed in 2009 and the results were re-checked in 2010. Tables of the cross-talk corrections are installed in the calorimeter software.
2. Joffe wrote the original package for the reconstruction of gamma conversions. The maintenance and update of this package has been taken over by the ATLAS e/gamma Working Group [Ref. A1].
3. Ishmukhametov developed specialized software to handle missing calorimeter readout channels due to failures of the optical data links for the 2010 data.
4. Hoffman coordinated software documentation for the ATLAS e/gamma Working Group. She ensures that all software package information used for physics analyses is current and relevant. This documentation is used by hundreds of users.
d) Electron identification (with Hoffman and Rios)

The study of electron identification was initiated in 2009 initially as the calibration of its energy using the Z boson signature and later in the context of Higgs decays to 4 leptons. Initial work emphasized enhancing the acceptance. Hoffman developed a method for the identification of electrons initially in the crack region between the barrel and end cap calorimeters and later within all edges of the detector. This method allowed for identification of electrons with incomplete showers or imperfect tracks and was incorporated into the general ATLAS software. It is maintained, improved and adapted to the changing run conditions by the e/gamma performance group. Further improvement was obtained by the introduction of a Gaussian Sum Filter (GSF)-based method to correct the electron trajectory for bremsstrahlung. The GSF uses a sum of Gaussian distributions to approximate the Bethe-Heitler distribution to model bremsstrahlung energy loss. Hoffman and Rios made numerous studies to validate the track parameters of electrons reconstructed using a GSF on data and MC. This resulted in better matching of tracks with calorimeter clusters and significantly increased electron identification efficiency [B2].
e) Photon Identification (with Joffe, Daya and Ishmukhametov)

Daya, Ishmukhametov and Joffe developed a measurement of the rate of electronphoton misidentification. The completely data-driven method relied on observation of a peak in the electron-photon invariant mass at the location of the Z pole. The misidentification rate was calculated from the magnitude of this peak, due to the fact that the "photon" came from misidentification of one electron in $\mathrm{Z} \rightarrow$ ee decay [A1]. This method has been used by Daya and Ishmukhametov for all photon spectra measurements in 2010-2012 and for the $\mathrm{H} \rightarrow \gamma \gamma$ searches. For early 2010 data the misidentification rate was found to be $\left(8.1 \pm_{\text {stat }} 2.0 \pm_{\text {syst }} 0.5\right) \%$. Initially, $86 \%$ of fake photons from electron misidentification came from the converted photon recovery procedure that resulted in objects being classified simultaneously as both photons and electrons. It was found that the high misidentification rate from photon recovery occurs predominately in those regions where there are dead or partially dead b-layer tracking modules in the detector. The misidentification rate has been further reduced in 2012 due to improved efficiency of the track-cluster matching for electrons using the GSF.

## Physics analyses

a) Measurement of the prompt photon cross section with the ATLAS detector (with Joffe, Daya, Ishmukhametov and Hadavand)

The measurement of the prompt photon and diphoton cross sections depends crucially on the estimate of the background due to fake photons. Daya and Ishmukhametov continued their work on electron-photon misidentification to calculate the impurity of the photon sample from electrons coming predominantly from Z and W decays. This provided a systematic error on the central value of
photon purity used to calculate the cross section. Ishmukhametov calculated the systematic uncertainty related to the loss in acceptance arising from the fact that photon candidates in problematic detector regions were not used in the analysis. To account for this effect in physics analyses, an object quality flag was assigned for each reconstructed electron or photon. This flag was based on the location of the core of the electromagnetic cluster of a given particle in relation to the dead or disabled detector region. For physics analyses done with direct electrons or photons, only particles passing object quality requirements were considered. The fraction of particles that are rejected due to this cut is usually calculated based on Monte Carlo samples of corresponding physics process, for which the object quality cut is also applied. Ishmukhametov studied the systematic uncertainty on applying MC based acceptance loss to the signal from data. He found this uncertainty to be on the level of 0.5\% for photons in early collision data. This work was documented in a number of ATLAS internal notes and presentations [A1-A11], was the basis of Ishmukhametov's Ph.D. thesis [A12], and was used in three publications [A13-A15].
b) Search for Higgs boson in the diphoton channel (with Daya and Ishmukhametov)

The technique of the data-driven electron-photon misidentification was also used for the search for $\mathrm{H} \rightarrow \gamma \gamma$ decays in the 2010 and 2011 data. Daya studied the contribution to the fully reducible background from the Drell-Yan process, where both electrons in the decay are misidentified as photons. This contribution was found to be $\sim 0(1 \%)$ of the total background. Ishmukhametov performed a Monte Carlo study of the effect of an increase in the photon energy resolution on the exclusion limit that can be set on the SM Higgs in the diphoton channel. To test this, the Higgs mass was reconstructed using photons that had their energies changed by $0.5 \%$ in one scenario and $1 \%$ in another. This procedure resulted in a "smeared" Higgs mass with broadened resolution. The effect on the Higgs exclusion was found to be a degradation of $8 \%$ of the expected limit. This work is documented in the ATLAS notes and conference presentations [C1-9] and the publication [C10]. It did not continue in 2012 due to graduations and departures.
c) Search for Higgs boson decays to 4 leptons (with Hoffman and Rios, Cao and Sekula)

The search for the Higgs boson in its decays to 4 leptons (electrons or muons) has been at the center of the group's attention for the past three years. Since a discovery is always made with the smallest number of events, the effort has been concentrated at maximizing the detection acceptance and efficiency and on the study of backgrounds. Hoffman and Rios took part in various tasks vital to the Higgs Working Group and had leading roles in optimization of electron identification, signal selection efficiency, and background rejection algorithms. These included managing the technical aspects of a cut-flow optimization and acceptance challenge, calculating final signal efficiency, systematic uncertainties for exclusion limits for both electrons and muons, and validation of an algorithm that accounts for the effects of bremsstrahlung on electrons (the GSF, discussed above).

To maximize the signal identification acceptance Hoffman and Rios studied in 2010 the cases where one or two leptons had been of a lesser quality or one of the leptons was in the forward region where there is not tracking information. For these " $2+2$ " and " $3+1$ " cases, where the second number refers to "imperfect electrons", the trade-off between the signal and the background was established. Many of the results were used to improve electron identification package that uses 32 parameters of the calorimeter signal shapes and track properties for the electron selection. For the 2011-2012 conferences, Hoffman and Rios continued analysis optimization and studied systematic uncertainties, trigger efficiencies, and Monte Carlo generator comparisons between PYTHIA and POWHEG for signal samples. They also coordinated an acceptance challenge for the group - ensuring the proper interpretation and application of selection criteria. In March 2012 they organized workshop that produced data selection criteria for the summer 2012 version of the analysis. For the discovery paper they estimated the systematic errors for the signal and background measurements and provided input to the global statistical analyses for Higgs mass exclusion ranges leading to eventual discovery of the Higgs signal.

This work resulted in a number of internal notes, paper and presentations at all major conferences in 2010-2012 [D1-D18], Rios' Ph.D. thesis [D19], and several publications [D20-D23]. The discovery paper has been published in [D23]. Hoffman has been an author on a substantial fraction of the supporting notes and was the coordinator and editor of the fermiophobic Higgs study. The searches culminated in 2012 with an unambiguous observation of the Higgs-like particle. The papers describing the discovery are listed in Ref [D24] for the 4-lepton final state and Ref.[D23] for the combination of all significant decay modes. The follow-up study of the spin-parity assignment of the new particle is given in Ref.[D25].


Figure 1: Plots for the summer 2012 data: left) The distribution of the four-lepton invariant mass. The signal expectation for a SM Higgs with $\mathbf{m H}=125 \mathrm{GeV}$ is also shown. center) Combined search results: (a) The observed 95\% CL upper limit on the signal strength as a function of $\mathbf{m H}$ and the expectation under the background-only hypothesis. (b) The observed local $\mathbf{p 0}$ as a function of $\mathbf{m H}$ and the expectation for a SM Higgs boson signal hypothesis. (c) The best-fit signal strength as a function of $\mathbf{m H}$. The band indicates the approximate $\mathbf{6 8 \%} \mathrm{CL}$. right) The ratio of the expected and observed $95 \%$ CL upper limits on the Standard Model Higgs boson production cross section.

In the fall of 2012, the results obtained for the Higgs decays to 4 leptons were combined with those for other decay channels leading to unambiguous discovery of the Higgs-like particle. The next obvious question was what is the spin-parity of this new particle. That has been best studied in the H->ZZ*->4 lepton decay final state where there are 5 observables describing angular distributions of the decays of each of the vector boson and relative arrangement of the decay planes. The results submitted to the 2013 Moriond conference [D24-25] showed a clear preference for the JP = 0+ assignment consistent with the expectations for the Standard Model Higgs boson.
d) Study of heavy bosons and search for a narrow di-electron resonance (with Daya and Ishmukhametov)

For the early data Daya and Ishmukhametov contributed to the observation of the W and Z bosons in the electron channel. They also participated in the measurement of the W and Z inclusive cross section measurements [I1-I4]. Later, Daya worked with Stroynowski on the searches for a high mass, sequential Z boson decaying into a pair of electrons. This was an effort of a large group of collaborators. Daya's work was concentrated on the detailed studies of electron identification performance for the data sample with two high $p_{T}$ electron candidates and the development of a datadriven method of estimating the "di-jet" background. Here, jets consist mostly of randomly overlapping electromagnetic showers from e.g., neutral pion decays with a charged pion track. This causes pion-electron misidentification. Other backgrounds are due to $t \bar{t}$ decays, WW, WZ and ZZ decays and the Drell-Yan process
[I5-I12]. The search for the signature of the sequential boson in the forwardbackward asymmetry of the decay electrons was the basis of Daya's Ph.D. thesis. [I13]

The di-electron spectrum showed excellent agreement with the estimated background. [I14-I15].


Figure 2: Dielectron invariant mass. Data points are shown in black. Various background estimates are shown in colors. The expectations for the sequential Z' bosons with masses of 1000,1250 and 1500 GeV are shown as unfilled colored histograms.

The data allowed us to set cross-section limits as function of Z' mass and these can be interpreted in terms of particular models. For the 2011 data these 95\% CL exclusions were: for the sequential SM-like Z' at $\mathrm{M}<1.83 \mathrm{TeV}$, and for an E6 modellike Z' at $\mathrm{M}<1.64 \mathrm{TeV}$.
e) Search for long-lived highly ionizing particles (with Firan and Ye)

The search for long-lived, highly ionizing particles was led at SMU by Firan. She originally designed the search for magnetic monopoles in her 2008 Ph.D. thesis [H1]. The signature of such a particle in ATLAS consists in the Inner Detector of track that has high-energy deposition due to ionization and manifests as a high fraction of TRT hits. The track is then matched with a narrow shower in the electromagnetic calorimeter.

This work was done together with groups from York and Oxford Universities and documented in Refs. [H2-H7].

The initial search was performed for massive, highly ionizing particles with lifetimes in excess of 100 ns (HIPs), using $3.1 \mathrm{pb}^{-1}$ of $p p$ collision data taken at $\sqrt{s}=7$. No events passed the selection criteria. Cross section upper limits between 1.2 pb and 11.5 pb have been extracted for HIPs with electric charges between $6 e$ and $17 e$ and masses between 200 GeV and 1000 GeV , were obtained under two kinematic assumptions: a generic isolated HIP in a fiducial range of $\eta$ and kinetic energy, or a

Drell-Yan fermion pair-production mechanism. In the resulting publication [H8] HIP mass ranges above 800 GeV were probed for the first time at a particle collider.

The signal of the magnetic monopole is characterized by a heavy ionization in its passage through matter and a trajectory that will bend in the $\mathrm{r}-\mathrm{z}$ plane but will be a straight line in the $\mathrm{x}-\mathrm{y}$ plane. The main effort of Firan for over two years was to correctly generate, simulate and propagate magnetic monopoles within the framework of the ATLAS Monte Carlo in order to obtain acceptance and efficiency for signal selection. She created and tested software package capable of generating magnetic monopole events with different masses and different magnetic charges for two production mechanisms: the Drell-Yan process and the two-photon process. This software became a part of the official MadGraph generator. For the detector response simulation and the propagation of the magnetic monopole through ATLAS, a new version of the GEANT G4Monopole package was created. This includes the correct propagation of a magnetically charged particle in the magnetic field present in the Inner Detector. A correction for the saturation effect due to high ionization in the material (Birk's Law) was calculated using the heavy ion collision data recorded by ATLAS. An analysis of $2 \mathrm{fb}^{-1}$ of 7 TeV data yielded no events passed the selection criteria. This allowed for the extraction of upper limits on the production cross section that extended to higher masses and significantly improved on the Tevatron limits. The paper published in Phys. Rev. Letters [H9].


Figure 3: Upper limits on the monopole production cross sections at 95\% confidence level. The solid line is the limit for single monopoles in the fiducial region and the dashed line is the limit assuming the kinematic distributions from Drell-Yan (DY) monopole pair production.

## f) Azimuthal Decorrelation in Dijet Events

The radiation of multiple quarks and gluons is one of the more complex aspects of perturbative quantum chromodynamics (pQCD). The proper description of radiative processes is crucial for a wide range of precision measurements as well as searches for new physical phenomena (SUSY, Higgs, etc.), where the influence of

QCD radiation is unavoidable or even for verifying various theoretical models. Hoffman and Rios, together with the BNL group, studied the azimuthal decorrelation, $\Delta \Phi$ of the leading (in $p_{T}$ ) jets in Monte Carlo simulation and data. In particular, they focused on two effects on the $\Delta \Phi$ distribution: when the z-position of the primary vertex was shifted by several millimeters, and and when there was an increase in multiple pp interactions per bunch crossing (in-time pile-up). In both cases, for the-amount-of data analyzed, the effects were negligible. Their work was part of a larger study that measured $\Delta \Phi$ in central high- $p_{T}$ di-jet events measured with the ATLAS detector. The main conclusion from the larger study is that results from an NLO pQCD calculation and from several Monte Carlo event generators provide a reasonable description of the normalized differential cross section. The results of this study were documented in the internal notes and conference papers [F1-F4] and published in Ref. [F5].
2.3.Ye (with Goldin, A. Liu, Xiang, Gong, K. Liu, Randle-Conde, Wang, Stroynowski, and Sekula)
a) Overview of past and current contributions

Ye is an experimentalist with the ATLAS collaboration. His primary recent work has been on detector readout. He supervises the research staff of the SMU OptoElectronic Laboratory. His work within the laboratory focuses on projects for ATLAS upgrades and for ATLAS operation. Ye's physics analysis effort has focused on two primary areas: the search for the Higgs boson via its $\mathrm{H} \rightarrow \mathrm{Z} \gamma$ decay channel and the search for a Dirac magnetic monopole.

Since 2011 Ye has been appointed the US ATLAS Level-2 manager for the Liquid Argon Calorimeter upgrade in which he works with groups from University of Arizona, Columbia University Nevis Lab, Brookhaven National Lab, Stony Brook University, University of Pennsylvania, and SMU. Ye is also the co-coordinator of the Joint ATLAS-CMS Opto Working Group that meets twice a year to address common issues in optical links in both experiments. One ATLAS-CMS common R\&D project, the Versatile Link (VL) [ $\mathrm{N}-6$ ], has evolved from this working group to develop radiation tolerant optical transceivers at $5 \mathrm{~Gb} / \mathrm{s}$ for the LHC upgrade. SMU is one of the three founding members in the VL collaboration. Collaborating with FNAL, ANL, UMN and OSU, SMU is leading the efforts in HEP to develop radiation-tolerant 10 $\mathrm{Gb} /$ s optical transmitters to answer the demands of $\mathrm{n} \times 100 \mathrm{~Gb} /$ s per front-end board in future HEP experiments.
b) Detector readout electronics and SMU's responsibility in ATLAS Operation:

Ye joined ATLAS in 1998, working with groups from CPPM, IPSC Grenoble, KTH, IPAS and SMU on the optical link system that reads out the LAr [ $\mathrm{N}-1$ ]. He later became the coordinator of this optical link group and led the project to its completion. In this project the SMU group gained valuable experience and expertise in high-speed serial data transmission over fiber optics for HEP experiments. We developed the capability to conduct irradiation tests on integrated circuits, optical transmitters and optical fibers [ $\mathrm{N}-2$ ], as well as system design and integration for fiber optics.

The LAr optical link system operates at $1.6 \mathrm{~Gb} / \mathrm{s}$ per fiber and has 1524 fibers with a total data bandwidth over $2.4 \mathrm{~Tb} / \mathrm{s}$. The transmitting side of the link resides inside the ATLAS detector. Hence it must withstand the significant radiation dose estimated for the 10-year operation at or above the design luminosity. This optical link is the state-of-the-art currently in use in HEP experiments. The SMU group (Ye together with the research staff and Stroynowski) has been responsible for this link system's maintenance and operation (M\&0) since the link's commissioning.

SMU was an integral part of the team that diagnosed and resolved one of the major challenges we have encountered in operating these links in the ATLAS Detector environment. The team was a task force led by the ATLAS electronics coordinator, and worked in close collaboration with groups in LAr and in other detector subsystems such as the Inner Tracker. It was observed that the optical transmitter (the OTx with a Vertical Cavity Surface Emitting LASER, or VCSEL) could sometimes fail. We investigated VCSEL failures caused by Electro-Static-Discharge (ESD) and by moisture in the ambient environment. Shown in Figure 5 is the VCSEL optical spectrum width (an indicator of the health of the device) subjected to different ESD. It is clear that the backward ESD does more damage to the emitting optical power. The ESD is introduced through a Human Body Model ESD circuit.


Figure 4: Optical spectrum of the VCSEL subject to ESD. The left plot lists results of forward ESD at $0 \mathrm{~V}, 500 \mathrm{~V} 700 \mathrm{~V}$ and 1100 V (from top down) while the right plot backward ESD at $0 \mathrm{~V}, 200 \mathrm{~V}, 300 \mathrm{~V}$ and 500 V .

The SMU group also conducted a life-test of one OTx operated in ambient air. As shown in Figure 6 below, the width of the VCSEL spectrum decreases with time, a clear indication that the OTx cannot operate stably with moisture in ambient air. This life-test is still ongoing at SMU with a large number of devices to gain statistical confidence.


Figure 5: VCSEL optical spectrum width as a function of time

We participated in the campaign of replacing all the optical transmitters that have weakened VCSELs with spares during the 2010 winter shutdown. Using the facility at SMU, we re-screened the spares with improved QA procedures. After this campaign, we no longer have problems with the OTx. The SMU group also provided a backup solution to this problem with the design of a new optical transmitter that has a redundant channel (the Dual-OTx), as shown in Figure 7. In the photo the Dual-OTx (top), which has the same electrical footprint as the OTx, is compared with one (bottom) that is currently in use.


Figure 6: Diagram and photo of the Dual-0Tx

This new design has been fully evaluated, and is now awaiting the collaboration's decision on a production to rebuild the spares. The SMU group is committed to the M\&O of the ATLAS LAr optical link system. By actively participate in the LAr upgrade program, this group maintains the expertise and equipment for high-speed serial data transmission, in particular over fiber optics, for HEP. This is vital for our commitment in the M\&0.
c) SMU's involvement in ATLAS upgrades and general R\&D for HEP
(i) The R\&D work on ASIC and components: As stated in the Letter of Intent to ATLAS, the phase-1 upgrade "will allow ATLAS to maintain low $P_{T}$ trigger thresholds for isolated leptons by increasing the granularity of the calorimeters involved in the Level-1 trigger". In this upgrade a new LAr Trigger Digitizing Board (LTDB) will be developed. Each LTDB will digitize calorimeter signals and send the digital information to the back-end via optical links with an aggregated data bandwidth above $200 \mathrm{~Gb} / \mathrm{s}$ per LTDB. A new data processing unit based on the FPGA architecture will also be developed to extract information for the Level-1 trigger.

The R\&D projects at SMU are supported by the US-ATLAS Operation to find solutions for the data transmission in the LAr trigger upgrade (phase-1) and for the whole LAr readout electronics upgrade (phase-2). In both cases we need optical links that withstand the LAr detector front-end radiation for the design luminosity and the expected operation lifetime after these LHC upgrade phases. The link's transmitting side must fit in the power dissipation constraint set by the existing cooling system, and must be highly reliable due to lack of frequent access for maintenance and repairing.

Other than this R\&D for a particular application, we are also supported through DOE's generic R\&D (Ye with BNL and Xiang with FNAL) to develop optical transmitters for future calorimeters. In these R\&D projects, plus the one that is supported by a DOE ADR grant (Ye, 2008-2010), we have identified a commercial 0.25 micron Silicon-on-Sapphire CMOS technology for ASIC developments in HEP [ $\mathrm{N}-3$ ]. This ADR project at SMU follows the efforts in DMILL, GaAs. It is in parallel to the evaluations in SiGe, the 0.25 and 0.13 micron CMOS technology carried out in the HEP community to study IC technologies for HEP experiments. Based on the SOS technology, we have successfully prototyped designs of a $16-\mathrm{to}-1,5 \mathrm{~Gb} / \mathrm{s}$ singlechannel serializer [ $\mathrm{N}-4$ ] and a 4.9 GHz phase-locked-loop for fast clock synthesizing
[ $\mathrm{N}-5$ ]. Shown in Figure 8 are the picture of the prototype chip $\left(3 \times 3 \mathrm{~mm}^{2}\right)$ and measured eye diagram of this serializer.


Figure 7: a photograph of the prototype chip which hosts the serializer, the phase-locked-loop (PLL) and several other designs. The 2:1 multiplexing unit in the serializer is visible in the upper left corner of the chip. In the lower right corner one finds the two wire loops functioning as inductors in the PLL. The eye diagram was measured at $5 \mathrm{~Gb} / \mathrm{s}$.

In June 2012, we submitted designs of a 2-channel array serializer, a single channel 50 Ohm VCSEL driver and an open-drain 4-channel array VCSEL driver, all designed to operate at $8 \mathrm{~Gb} / \mathrm{s}$ per channel. This represents the highest speed of such data transmission ever designed in HEP. The layout of this prototype chip is shown Figure 9. The test of these designs will start in 2013.


Figure 8: layout of the prototype chip submitted in June 2012. The 2-channel array serializer with its PLL clock unit takes most part of the chip area. The laser drivers are on the right side of the chip, with the 4-channel array VCSEL driver visible in the lower right corner

As mentioned above, the SMU team is collaborating with FNAL and several other US institutions to develop $10 \mathrm{~Gb} / \mathrm{s}$ per channel radiation-tolerant optical transmitters to meet the challenges of high data rates in future detector front-end readout. In this R\&D project, SMU takes two approaches, one based on TOSA (packaged VCSEL or Transmit Optical Sub-Assembly) and the other based on array optics, to strike a balance among constraints in channel and system reliability, power consumption and heat management, optical coupling efficiency, and cost. In the same line of optical link developments and in the framework of the Versatile Link Common Project, we collaborate with a group in Oxford, UK (ATLAS Inner Tracker) on fiber and passive component identifications and evaluations [ $\mathrm{N}-8$ ]. In the VL project, SMU is responsible for studies that provide link system level design guidelines [N-7]. All of these efforts have already been proven to be helpful and cost-saving in the particular optical link design for LAr phase-1 upgrade.
(ii) Ye's responsibility as the US ATLAS Level-2 manager: as a managerial duty Ye works closely with US and international institutions that are interested and contributing to the LAr upgrades, in particular the phase-1 LAr trigger upgrade. The US institutions lead the efforts to upgrade the front-end by designing a full digital trigger board. The US is also a key player in developments for the back-end electronics. SMU takes sole responsibility for the transmitting side of the optical link system, and works with European collaborators on the link's receiving end. All these R\&Ds involve component or subsystem developments such as the analog front-end (UPenn, BNL), the analog to digital converter ASIC (Nevis), the LOC ASIC, the optical data link and the GBT, VTRx based control link (SMU), and the back-end FPGA based data processer (UAZ, BNL, and SUNYSB); they also involve system level design and demonstration. In March 2012 at SLAC the US LAr team in the upgrade had an internal review in which the reviewing committee commended the efforts and achievements of the team. We are on-track in preparation for CD reviews and for a construction phase starting in 2014. On the international side, the LAr collaboration is aiming for an ATLASTechnical Design Review in mid-2013. From a technical standpoint, we plan to construct a full-scale demonstrator system (front- and backend boards and the optical link between them) with ASICs and COTS, and install the demonstrator LTDB inside ATLAS during the 2013-14 shutdown (the LS1) period. This demonstrator will be a vital step from which we gain experience and guidance in components and system developments towards the final installation during the 2018 shutdown (the LS2). Prioritized by US-ATLAS, projects in the phase-1 LAr trigger upgrade are on-track.
(iii) SMU in LAr phase-1 upgrade: SMU plays an important role in the LAr phase-1 upgrade. Ye with his group is responsible for developing the SOS based LOC ASIC chipset (several designs), and the optical data link that transmit digitized trigger data from the front-end LTDB to the back-end sPU, which is the FPGA-based super Processing Unit that provides processed information for the Level- 1 Trigger. We
also develop the GBT, VTRx-based control link that provides clock, configuration, control and monitoring to the front-end electronics. The LTDB will replace the function of the present analog Trigger Tower Build Board (TBB); the control link will replace functions that are currently provided by two boards in the front-end crate: the Controller Board and the Monitoring Board. The data rate from one LTDB will be above $200 \mathrm{~Gb} / \mathrm{s}$, 2 orders of magnitude higher than the current state-of-art: $1.6 \mathrm{~Gb} / \mathrm{s}$ from one Front-End Board (the FEB) in LAr.

Aside from difficulties in high data rate and in the radiation tolerance requirement from the increased design luminosities of the LHC upgrade, challenges in this upgrade also come from constraints such as the cooling capacity that will be kept unchanged. For example, with more than 100 times increase in data rate, the power dissipation budget to the optical link will only be allowed to increase by a factor of 10. In these regards, we have successfully prototyped ASIC designs that will meet the requirements for the upgrade. We are also working on a few final prototypes that will lead us towards the packaged IC chips that will be used in the optical link of the LTDB.
d) Physics analyses with ATLAS data:

Searching for Dirac magnetic monopole (Firan, Stroynowski, and Ye): This work was a collaborative effort within the SMU ATLAS group and was described in section 1.2e.

Searching for Higgs via $\mathrm{H} \rightarrow \mathrm{Z} \gamma$ final states (Goldin, Randle-Conde, Sekula, Wang, and Ye): Ye initiated this work at SMU with postdoctoral fellow Daniel Goldin. This is a channel that may contribute to the search for Standard Model Higgs with decays into $\gamma \gamma$ and ZZ (4 leptons final states), it may also probe physics beyond the SM should an enhancement in the number of events be observed in data. Such an enhancement might indicate new particles in place of the W and Top loop.

Goldin carried out MC studies that include the feasibility of Higgs associated production with a Z or a W in which the Higgs decays into $\mathrm{H} \rightarrow \mathrm{Z} \gamma$. Goldin's work stopped for lack of data and he later moved to a Tevatron experiment with a different institution. In early 2012 this work was resumed at SMU with Aidan Randle-Conde (postdoc), graduate students and later joined by Hulin Wang (postdoc starting in August 2012). Sekula, Ye and Stroynowski are also active in this search. Although the branching fraction for the $\mathrm{Z} \gamma$ final state is similar to that for Higgs
decay to two photons, the background from QCD mediated decays are more severe and the limits obtained in the search done so far have been about a factor of 6 larger than those predicted by the Standard Model.

### 2.4. Kehoe (with Hadavand, Dindar, Kama, Kasmi)

Kehoe studies the mechanism of electroweak symmetry breaking primarily through the measurement of the top quark mass and the search for the Higgs boson in diboson events. Significant contributions in jet energy calibration and trigger and data quality (DQ) software support this effort. ATLAS Higgs studies leverage D0 top research, partly via common signatures and analysis techniques.

ATLAS Detector Operations:
Thousands of cores in the High Level Trigger (HLT) execute trigger and monitoring algorithms using a modified ATLAS Athena framework. Since 2005, Kehoe led a US ATLAS project developing key elements of the monitoring side of the trigger system, including the DQ Monitoring Framework (DQMF) with UC Irvine, and the Gatherer. In 2010, Kehoe and Sekula formally joined TDAQ as a group at SMU. Kehoe now focuses on the challenges posed for by multi-core CPUs and 64-bit software, which requires redesign of the core Trigger software.
a) Data Quality (Hadavand, Renkel, Kama, Kehoe, Kasmi): SMU develops the central online application, 'Gatherer', that employs a variety of algorithms to centrally sum or merge monitoring output for final DQ. Renkel maintained Gatherer and implemented several improvements such as allowing fine time granularity down to one luminosity block. Kama took over development in late 2010 and upgraded its interaction with ATLAS Run Control. Renkel, Kasmi and Kehoe developed a software test bed that established the acceptable CPU and memory performance of the Gatherer and its scalability for increased numbers of histogram providers. Later tests by Kama in new HLT nodes pointed to future scalability challenges. Partly due to this exercise, Kama developed with Kehoe, Renkel and Hadavand a proposal for a new 'MonInfoGatherer' (MIG) application. The designed framework splits the control structures from information handling and summation methods. The latter is exposed as an API that enables gathering as a plug-in for other applications. This greatly enhances scalability when many-core processors are used by enabling gathering within each HLT node. The framework approach also provides easy extensibility, letting custom containers and summation methods to be easily implemented. Kama presented this proposal at a TDAQ Software week and implemented MIG in stages. A fully functional MIG has been included in TDAQ releases and is recently running at Point1 in parallel with the monolithic Gatherer. Side-by-side tests indicate similar performance in the current HLT, while MIG has the plug-in capability needed for the future.

SMU Calorimeter monitoring continued in 2010 with development by Hadavand of improved Athena algorithms for reconstructed topological clusters, towers and cells, including monitoring of jets from CaloTowers. Her tools were used by CaloGlobal, LAr, Tile and Jet/Etmiss shifters for final DQ sign-off, and she and Kehoe took shifts during the period. She also maintained and updated the package of DQ algorithms used in DQMF [M.9] including adding helper algorithms to facilitate development in online and offline contexts. Kama performed code inspections of the important HistMon and OHP services. DQ is performed in Tier0 using DQMF connected to offline-specific services, including a web-based display used by all offline shifters. Kama took over web-display development in 2010/2011. He improved stability and incorporated many new features, including flexibility to choose histograms by stream or run. Kama was the primary on-call expert for the offline DQ which was a major responsibility to maintain the operation and software of the system. He made several substantial improvements, including easing DQ configuration, improving DQ application task management, bookkeeping and improving speed and efficiency of DQ production, and automating error reporting to experts. Kama supported users during this time, creating an archived DQ help mailing list and arranging a Good Monitoring Practices Workshop. His work greatly improved the stability of the offline DQ. The contributions of several SMU members who built and operated various elements of the DQ were key to the rapid ability to analyze new data for the recent Higgs observation.
b) Trigger Core Software and Performance Optimization (Kama):

ATLAS software must be restructured to take maximum advantage of current and future hardware architectures. Current challenges include implicit serialization of processing, or lack of vectorization. Following our efforts on Gatherer performance, Kama was asked to test reconstruction algorithms. He identified to the developers two bottlenecks where reordering the objects in memory would reduce cache misses, and vectorization of calculations reduce CPU stalls. He currently serves as the TDAQ representative to the A-Team which pursues solutions for these kinds of challenges. Multiprocessing overcomes the limitation posed by highly multi-core processors. To facilitate multiprocessing in the HLT ('HLTMP'), Kama works with the new implementation of a multiprocessing Athena ('AthenaMP') from the ATeam. He created a new set of packages including a HelloWorld application and a test bed for HLTMP implementation. The results confirmed the potential of using MP in the online environment and observed memory sharing was compatible with offline AthenaMP. The Data Flow evolution includes the 'HLTPU' application which incorporates the function of both Level 2 and Event Filter. Kama implemented a dummy multiprocessing HLTMPPU that simulates an HLTPU by consuming CPU similarly to real event processing which is necessary for testing TDAQ. He is now co-convenor on the TDAQ side of a new Future Software Technologies Forum for a broad discussion of computing solutions for Phase 0 through 2 upgrades.

ATLAS Physics Analyses:


Figure 9: Background-subtracted $m_{T}$ distribution in ATLAS $1 l+E_{T m i s s}$ events

Kehoe studies diboson (VV) events with a goal to search for the Higgs boson. This started in 2007 with searches in diphoton events for evidence of extra dimensions because LHC gives a dramatic increase in sensitivity over the Tevatron, even at modest integrated luminosity. To provide broad search sensitivity to the Higgs mass and to enable possible study of Higgs properties, however, he focused on the search for Higgs $\rightarrow \mathrm{WW} \rightarrow \mathrm{l} v \mathrm{l} v$. Such a search also shares many attributes with Kehoe's study of $t \bar{t}$ pairs at the Tevatron.
a) Extra Dimensions in 2g Events (Hadavand, Dindar-Yagci, Kehoe): We collaborated in the search for evidence of Universal Extra Dimensions (UED) in $\gamma \gamma^{+}$ $\mathrm{E}_{\text {Tmiss }}$ events in the first $3 \mathrm{pb}^{-1}$ of 2010 data. Dindar and Kehoe performed several comparisons of data with the total expected background in background-rich control regions. A template fit yielded the first accurate estimate of photon purity in the MC background sample [K.1]. Dindar tested different background normalization methods and the effect of pileup. Her comparisons and $c^{2}$ calculations were a focus of the Editorial Board (EB) and necessitated a final systematic uncertainty. Hadavand worked on identifying an optimal event selection and led many cross checks of expected event yield vs. event selection step that were important during group review. She studied the high $\mathrm{p}_{\mathrm{T}}$ photon efficiency to provide systematic uncertainties when the background was extrapolated into the signal region, and to provide one due to dead OTX's. Hadavand was interim editor and convenor when the primary coordinator was absent. No signal was observed and the limit exceeded the Tevatron's [K.2].

We searched for the RS graviton with the first $36 \mathrm{pb}^{-1}$, which our earlier studies showed to be competitive. Hadavand continued her emphasis on photon efficiency and OTX systematics from the UED analysis. This helped her optimize the estimation of background in the signal region. She and Dindar demonstrated that loosening the identification would maximize significance while keeping background in control. Dindar and Kehoe completed a study of the impact of coupling $\left(k / M_{p l}\right)$, which specifies the graviton width, and mass ( $\mathrm{M}_{\mathrm{G}}$ ) on signal distributions to develop a signal model. Hadavand developed a frequentist unbinned maximum likelihood fit using signal and background parametrizations. She guided Dindar to finish the implementation of this method for her dissertation [K.5], including parametrization of the signal. The resulting limit was slightly higher than the published method and surpassed the Tevatron sensitivity for $\mathrm{M}_{\mathrm{G}}>1 \mathrm{TeV}$ [K.4]. We followed this with analysis in $2.12 \mathrm{fb}^{-1}$. Hadavand contributed to the treatment of background
kinematic shapes, use of pseudoexperiments in testing the analysis performance, and making the use of PDFs more consistent. She implemented at SMU the Bayesian Analysis Toolkit used by the dilepton analyses and extracted limits. She also led the way to identify and resolve inconsistent results from different fitting methods. Hadavand was editor of the analysis support note [K.3], and co-editor of the paper. No signal was observed and the resulting limit is $\mathrm{M}_{\mathrm{G}}>0.8 \mathrm{TeV}$ for $\mathrm{k} / \mathrm{M}_{\mathrm{pl}}=0.01$ [K.6].
b) Search for Higgs $\rightarrow$ WW (Kehoe): Kehoe focused on the production of VV backgrounds for the Higgs search. This entailed overlapping work in the Higgs and SM WW groups. Kehoe worked on the determination of the WW cross section in 7 TeV collisions with technical assistance from BNL to get started. He performed the first estimation of the internal conversion $\mathrm{Wg}^{*}$ background using recently available MadGraph D3PDs, which showed this background to be at least as large as the Wg background. At the time, an NLO calculation was not available to obtain the normalization, so Kehoe compared the kinematics of Alpgen Wg and MadGraph Wg* events. He demonstrated the $\mathrm{g}^{*}$ mass ( $\mathrm{m}_{\mathrm{g}^{*}}$ ) spectrum was extremely low, even after event selection cuts, resulting in leptonic kinematics very similar to Wg . These results motivated preliminarily using the $k$-factor from Wg events in the 0 -jet bin with a large uncertainty. He also estimated the overlap of $\mathrm{Wg}^{*}$ and WZ processes. Kehoe coordinated with students from Michigan to estimate the other diboson backgrounds (WZ, Wg, ZZ), and he did the final calculation of combined statistical and systematic uncertainties. Kehoe wrote the VV background and MC portions of the SM WW support note [I.16] , the basis for presentation at Moriond [I.17]. In parallel, he presented his work on $\mathrm{Wg} / \mathrm{g}^{*}$ to the Higgs $\rightarrow \mathrm{WW}$ subgroup and contributed to that group's Planning document for 2012 analysis [E.1].

He focused in the $\mathrm{H} \rightarrow \mathrm{WW}$ group putting the $\mathrm{W}->\gamma^{*}$ on a better footing and on ensuring sufficient MC samples existed. In the former case, he studied filter thresholds so new Alpgen Wg samples greatly reduced the statistical error while being fully efficient. Kehoe's comparison of Pythia 6 and Pythia 8 variants of these samples demonstrated a problem with the Pythia 8 production so this showering was not used for final analysis. To normalize $\mathrm{W} \gamma^{*}$, Kehoe studied the correlation between $\mathrm{m}_{\mathrm{g}^{*}}$ and event kinematics. To compare with LO MCFM calculations by colleagues at Oxford and Roma Tre, he determined LO MadGraph cross sections under different mass and kinematic selections. The MCFM NLO calculation was unstable when $\mathrm{m}_{\mathrm{g}}{ }^{\lll} 1 \mathrm{GeV}$. Kehoe worked with colleagues to establish a mass range and kinematic selection from which to determine NLO cross sections. His observation of the independence of event kinematics on $\mathrm{m}_{\mathrm{g}^{*}}$ if $\mathrm{m}_{\mathrm{g}^{*}}<$ few GeV was instrumental in convincingly extrapolating a normalization for $\mathrm{m}_{\mathrm{g}} \times 0.5 \mathrm{GeV}$ into the lower mass range. A systematic uncertainty was extracted from these studies. In addition to use in the $\mathrm{H} \rightarrow \mathrm{WW}$ analysis, Kehoe ported these results and samples to the final 7 TeV SM WW cross section analysis where he repeated his VV calculation and editing roles [I.16, I.18]. He estimated several contributions to be negligible in $\mathrm{H} \rightarrow$ WW EB review: $\tau$ decays, photon FSR, and $\mathrm{W}+\mathrm{J} / \psi$ background. Kehoe was co-
editor of the $\mathrm{H} \rightarrow \mathrm{WW}$ Theory supporting note [E.2]. Upon unblinding, a 3.3s excess above background was observed with a $l l+E_{T m i s s}$ transverse mass ( $\mathrm{m}_{\mathrm{T}}$ ) distribution (see Figure 10) [E.2-7]. This contributed to the ATLAS total 5.9s observation of what appears to be the SM Higgs boson [D.23].

Kehoe also performed a study detailing differences in modeled jet multiplicity between $\mathrm{W} \gamma$ and $\mathrm{W} \gamma^{*}$ events. This was used in the systematic uncertainty for the discovery analysis, and was the basis for the reweighting approach developed in fall. Further efforts involved working with Oxford colleagues on a scheme by which Sherpa was used to model very low mass diphoton pairs. These results were presented in updates at HCP 2012 and Moriond 2013. Kehoe remained as Theory note editor, and was appointed as co-convenor of the Theory group.

Kehoe also joined the Snowmass effort to work on projections for ttH production with emphasis on $\mathrm{H} \rightarrow \mathrm{WW}$. He worked on the initial signal-to-background estimates with U. of Texas colleagues, and co-organized a Snowmass workshop on the topics. He convened a preliminary meeting in March and summarized the results and status from several groups at the April Energy Frontier meeting at BNL.

Other ATLAS Activities (Dindar, Kasmi, Kehoe with Stroynowski): The jet energy scale (JES) is important to many analyses in proton collisions. Kehoe continued an earlier JES role to prepare the report as Chair of the Review Panel for the 2009 Hadronic Calibration workshop, and to coordinate the $\gamma+$ jet session of the 2010 Pisa workshop. This placed $\gamma+$ jet as an important component of the ATLAS JES [M.10]. Kehoe advised Kasmi in the context of the wider SMU effort as he finished his analysis and dissertation on ZZ and $\mathrm{H} \rightarrow \mathrm{ZZ}$ production using topo-clusters and no tracking [I.19].

### 2.5. Sekula (with Cao, Randle-Conde, Wang, and Ye)

Sekula joined the SMU ATLAS group in 2009. Since then, he has become involved in work on the ATLAS trigger, simulation of the ATLAS trigger upgrade, and data analysis. He has earned increasing leadership roles in the physics analysis community. His primary interests are in the search for additional Higgs bosons in nature, the understanding of the properties and implications of the new state at 126 GeV , and in the effect of increasing luminosity and pile-up on trigger performance and response. These and future plans are all described below.

ATLAS Operations and Technical Work
In addition to trigger desk shifts in the ATLAS Control Room and remote data quality shifts, the primary contributions of Cao, Randle-Conde, and Sekula have been to the ATLAS TDAQ effort. These are described below.

## a) Predicting pileup effects on ATLAS trigger rates (Cao, Randle-Conde,

 Sekula)Our key technical contribution has been to understand how increasing luminosity, and thus increasing proton-proton collisions per bunch crossing ("in-time pile-up," henceforth referred to as "pile-up"), will affect ATLAS trigger rates. We have focused on developing predictive mechanisms. This information helps many members of ATLAS involved in routine operations, from the ATLAS Trigger Menu Group to the Trigger Desk Shifter, make informed decisions about alterations to trigger prescales and the trigger menu; such changes can have profound impacts on all aspects of physics analysis.

The number of pile-up collisions occurring at a given luminosity is a Poisson process, centered on a mean value given by $\mu=(L \sigma) /(f N)$, where $L$ is the instantaneous luminosity, $\sigma$ is the cross-section



Figure 10: (top) The integrated ATLAS luminosity in each year, 2010-2012. (bottom) The average collisions per bunch crossing. for proton-proton interactions, $f$ is the bunch frequency, and $N$ is the number of colliding proton bunches. For instance, for typical operating conditions present in early 2012 ( $\mathrm{L}=6 \times 10^{33} / \mathrm{cm}^{2} / \mathrm{s}$ ), $\mathrm{N}=1380$, $\mathrm{f}=11,245 \mathrm{~Hz}$, and $\sigma_{\mathrm{pp}}{ }^{\text {inelastic }}=70 \mathrm{mb}$ ) this meant a mean number of pile-up collisions was typically expected to be $\langle\mu>=27$, in good agreement with the measured values shown in alterations to trigger pre-scales and the trigger menu; such changes chave profound impacts on all aspects of physics analysis.

## b) Prediction of trigger rates with increasing pile-up (Randle-Conde, Sekula)

Postdoctoral fellow Randle-Conde has played a key role in predicting trigger rates with pile-up in the ATLAS Trigger Rates Group. Sekula initiated this project within the ATLAS Trigger Rates Group in 2010, and in 2011-2012 Randle-Conde was the leading contributor and developer of this predictive mechanism and framework; since 2011, others have become involved in aspects of the project, including Graduate Student Cao.

The importance of accounting properly for pile-up effects on trigger rates is illustrated in Figure 11 for one of the more challenging Level-1 triggers: the missing
energy significance. We see that without including the pile-up effects in trigger rate scaling, it is impossible to make reasonable predictions for the behavior of the trigger across a run (divided into luminosity blocks). Work has continued over the 2011-2012 running period and key triggers, including electromagnetic and missing energy triggers, can all now be predicted to within a few percent of the true value as a function of time during a run.

The importance of understanding trigger scaling cannot be understated. Deviations from the predicted trigger rate have been used to diagnose problems in ATLAS subsystems. For instance, recent running in the spring of 2012 saw the advent of high trigger rates due to electronics problems in one of the subsystems. The problem was observed by noting the difference from the expected trigger rate for a given set of running conditions, and then quickly reported to the subsystem and the Run Control shifter in the ATLAS Control Room. In addition, the Trigger Menu Group uses this information to decide on pre-scales and how they will be


Figure 11: A comparison of trigger rates for a particularly challenging trigger - the Level-1 computation of missing energy significance. Without a correction for pileup effects, we see that ATLAS is essentially unable to make any reasonable rate prediction. altered during running conditions to maximize data-taking and minimize dead-time.

This work has become routine and is expected to continue through the end of datataking in 2013. Other activities, described below, are then expected to become a central focus of Sekula's trigger work.

## c) ATLAS Control Room Trigger Desk Prediction vs. Measured Trigger Rate Monitoring (Cao)

Graduate student Cao began her contributions to the ATLAS Experiment in the fall of 2011, initiating a project to connect the trigger rate predictions to the Trigger Rate Presenter (TRP), a tool commonly used by both online Trigger experts and the ATLAS


Figure 12: The Trigger Rate Presenter showing Graduate Student Cao's framework for displaying rates, predictions, and comparison flags.

Control Room Trigger Desk Shifter to diagnose and resolve trigger issues.

Cao's project was to develop software adapters to deliver information needed for trigger rate prediction (obtained from online databases) to the TRP. This would allow the TRP to display predictions for the Level-1, Level-2, and Event Filter trigger systems. These predictions could then be compared to the actual rates, also displayed in the TRP. Cao's software was designed to summarize the prediction and its comparison with the real rate using a "flag" - she chose to use the number of standard deviations ("nSigma") between the prediction and the real rate. This allows the shifter to then sort the table of trigger lines by their nSigma values and isolate those with the largest deviations. Her finished project is shown in Figure 12; while much of her effort was the development of software "behind-the-scenes," the TRP panel is the visual conclusion to her work. This effort was well-regarded by both the ATLAS Trigger Online group and Trigger Rates Group.

## d) Trigger Upgrade Studies - Physics Impacts (Cao, Sekula)

The trigger is expected to undergo several upgrades during the lifetime of the ATLAS Experiment. Efforts are currently underway to develop "topological triggers" for the Phase 1 ATLAS Upgrade; rather than focusing on just the kinematics of single objects or object pairs, these triggers would focus on the angles and energies of multiple objects. In addition, efforts to develop a track trigger are underway and there is a plan to expand the Level-1 readout granularity of the calorimeter for Phase 2. While the physics impacts of the

Super-Cell definition


Figure 13: Definition of a Trigger "Super Cell," needed for high-granularity calorimeter readout studies. topological triggers are being wellstudied within ATLAS, there is still the question of the physics impacts of upgrades like a track trigger or a higher-granularity readout from the calorimeter.

Sekula began the study of increased calorimeter granularity on tau triggers in 2011 and came to some preliminary conclusions in 2012. Using what were then considered "very high-pileup" simulations samples with an average of 46 protonproton collisions per crossing, Sekula studied the possibility of using high-level tau identification variables in hardware at Level-1. The goal was not to define the hardware specifications needed to implement such a scheme, but rather to focus on whether such a scheme has a positive and meaningful physics impact.

These efforts narrowly focused on the question of whether or not a highergranularity calorimeter readout in the Level-1 trigger would allow for better discrimination of hadronic tau decays from quark and gluon jets. The parameters of such a higher-granularity readout are illustrated in Figure 13. The current trigger reads out the calorimeter in $\Delta \eta x \Delta \phi$ regions of size $0.1 \times 0.1$, which is about four times the area occupied by a single calorimeter cell ( $0.025 x 0.025$ ). Sekula investigated what would happen to tau triggers if one could read out the calorimeter using "Super Cells" (Figure 13), which are of size $0.025 \times 0.1$. This allows a more fine-grained definition of energy distribution variables, including the energy occupied by the core of an electromagnetic cluster ("Reta") and the isolation energy (the energy in a ring around the cluster).


Figure 14: the fraction of total energy in a ring around the central cluster core (Isolation Fraction). This was computed using energy in trigger Super Cells.

Using a 1 GeV energy digitization scale, Sekula and Cao defined these variables and used simulated samples of jets and highpT tau leptons to see how well they could be separated while keeping the Level-1 pT thresholds as low as possible. The overall goals of this study were to select taus with a sufficiently high efficiency (90-98\%) while also keeping the single-tau trigger within a 20 kHz rate budget for the overall trigger. An example of one of these variables, the "Isolation Fraction" (the ratio of energy in a ring around the central cluster core to the total energy of the cluster) is shown in Figure 14.

The conclusions of this preliminary study were promising, but raised a number of new questions that still need to be addressed. We found that if we could define such energy shape variables in the Level- 1 trigger, we could reduce the trigger rate by $40 \%$ while maintaining a lower pT threshold and a tau trigger efficiency of $90 \%$. However, a $40 \%$ reduction was not sufficient to achieve the goal of maintaining the tau trigger rate at 20 kHz . The best trigger rate we could achieve for a still-low pT threshold was for $\mathrm{pT}>40 \mathrm{GeV}$, and that rate was 40 kHz - still a factor of 2 too high to be reasonable for a future trigger scenario.

## e) Future Directions in Tau Trigger Studies

The ATLAS upgrade physics impact study raised important questions that need to be addressed:

The study was done using ROOT files, and rebuilding trigger towers from a combination of current Level-1 "Regions of Interest" and the calorimeter cells present in those regions. This is not how a future trigger would work. It would,
instead, START from Super Cells and define trigger towers and regions of interest. To address this problem, the study needs to be done by first implementing highgranularity software tools into ATLAS ATHENA so that ROOT files with the full trigger simulation using Super Cells can be produced. This is a significant amount of software work and was not possible in 2012 due to other commitments.

The study was done using a 1 GeV digitization scale for Super Cell energy. However, it's necessary to explore other scales ( $0.25 \mathrm{GeV}, 0.5 \mathrm{GeV}$, for instance). These may allow for better control of the long tails seen in the energy shape variables computed using the Super Cells.

A new effort is required determine how a future track trigger and a highergranularity calorimeter readout might work together to enhance hadronic tau triggering at Level-1. This is a fruitful but unexplored area of the project, and would require significant time investment to advance it.

The goal is to restart work on this area in 2012-2014 during the end of data taking and the long shutdown period. We envision a postdoctoral fellow taking the lead in this effort.

## ATLAS Physics Analysis

a) The measurement of $\mathrm{H} \rightarrow \mathrm{Z} \gamma$ (Randle-Conde, Sekula, Wang, Ye)

This measurement effort was described earlier, in section 2.4b, and is a collaboration within the SMU ATLAS group.
b) The Search for an Electrically Charged Higgs Boson ( $\mathrm{H}^{ \pm}$) (Randle-Conde, Sekula)

The discovery of a particle that is so-far consistent with the Standard Model Higgs Boson has raised a number of important questions for the field. Kehoe, Sekula, Stroynowki, and Ye are all invested in measuring the properties of this new particle by understanding its decay modes and decay rates, as well as its spin and CP quantum numbers. In addition to this critical effort, Sekula is advancing the frontier of the search for additional Higgs bosons in nature.

The existence of Dark Matter is a challenge to the Standard Model. If Dark Matter is composed of particles, those particles are not described by the SM. If the Higgs mechanism is the means by which subatomic particles acquire mass, then we are left with a key question: what Higgs boson gives mass to the Dark Matter? The SM Higgs boson is an insufficient answer to this question, as it has only enough couplings to give mass to the particles described by the SM. The search for additional Higgs bosons now takes on more urgency, and Sekula is leading an effort to find an electrically charged Higgs boson.

There are many popular extensions of the SM, most of them based in the framework of supersymmetry. In any of these extensions, at least one new Higgs field doublet is added to the SM Higgs doublet; this results in at least 5 physical Higgs boson states, two of which are always electrically charged. The observation of an electrically charged Higgs boson would be unambiguous evidence of physics beyond the Standard Model.

In addition, a decade's long effort by the B-Factories, BaBar and Belle, has yielded branching fractions for the decays $B \rightarrow X \tau^{ \pm} v$ which have strong tension with the SM predictions. Here, "X" can be either nothing or a charm meson (e.g. D or D*). The same tension is simply not present for the decays of charm mesons to these taulepton final states. This suggests that heavy flavor decays to heavy lepton final states are not well-described by the Standard Model, leaving room for contributions from a charged Higgs boson.

## Search for a low-mass $\mathbf{H}^{ \pm}$using $t \bar{t} \rightarrow W^{+} b H^{-} \bar{b}$




Figure 15: (left) the MET distribution fitted using a QCD and non-QCD template. (right) The final composition of the 2011 data, with signal overlaid.

## c) Light charged Higgs production and decay (Randle-Conde, Sekula)

The ATLAS Collaboration created a special Higgs subgroup, HSG6, in 2011 solely for the purpose of advancing the search for the charged Higgs. Randle-Conde and Sekula had become involved in this search in late 2010 and were among the first members of the ATLAS Collaboration to study, in a data-driven way, the backgrounds that would be a challenge to this search. Our focus was on the production of top pairs and their subsequent decay to the following final state:
$t \bar{t} \rightarrow W^{+} b H^{-} \bar{b} \rightarrow(j j) j_{b}\left(\tau_{h} v\right) j_{b}$
where " j " denotes a light-quark jet, "jb" denotes a bottom-quark jet, " $\tau_{\mathrm{h}}$ " denotes a hadronically decaying tau lepton, and the neutrinos in the final states of the $\mathrm{H}^{ \pm}$and
the tau decays manifest as missing transverse energy (MET). This "all-hadronic" mode is attractive in that it accesses a large portion of the possible final states of decay (the hadronic branching fractions of the W and the $\tau$ are typically twice as large as the leptonic branching fractions). However, the mode at first appears to be a significant challenge due to the presence of only hadrons in the final state.

Sekula and Randle-Conde were responsible for significant portions of the analysis. SMU took a lead role in developing the baseline cut selection, the QCD background estimate, and the evaluation of systematic uncertainties. In addition, Sekula was appointed by the HSG6 subconvener to be the analysis leader of the allhadronic final state effort, and was selected as one of three co-editors for the publication (one from each channel used in the search). The final publication included three independent topologies in the search: the all-hadronic topology (denoted "tau+jets") and two lepton-based topologies ("tau+lepton," accounting for leptonic W decays, and "lepton+jets," accounting for leptonic tau decays).

Randle-Conde's primary contribution was the measurement of the QCD background. The key variable at the end of this analysis is the "transverse mass" of the tau and missing energy system, computed using
$m_{T}^{2}=p_{T}^{\tau} E_{T}^{\text {miss }}(1-\cos \phi)$, where $\phi$ is the angle in the transverse plane between the tau momentum and the MET. This variable has a threshold at the mass of the parent particle; if the tau and MET arise from a W boson, this distribution has a threshold at the W mass. Multi-jet QCD background


Figure 16: (left) the model-independent $95 \%$ CL exclusion on the brancl (right) The MSSM exclusion in the mh-max scenar contributes to the distribution in a way that must be determined from data, as simulation of this background is usually (1) unreliable and (2) of insufficient statistical significance to draw conclusions. Randle-Conde developed a data-driven method where he inverted the tau lepton identification and required that events have no b-tagged jets in them. This produced a subsample enriched in QCD background, from which a template of the MET shape could be made. This template could then be fitted to the nominal MET shape in our signal sample to determine the fraction of the MET distribution occupied by QCD background. Finally, the QCD fraction could be fixed from the fit and the transverse mass QCD contribution determined. All of this is illustrated in Figure 15. These results appeared in a series of conference notes and internal ATLAS notes [L1-L4], culminating in the first ATLAS publication on the subject in spring 2012 [L5]. The published results were also presented by Randle-Conde and Sekula at conferences [L6-L7].

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# Search for the Standard Model Higgs boson in the two photon decay channel with the ATLAS detector at the LHC ${ }^{\text {N }}$ 

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#### Abstract

A search for the Standard Model Higgs boson in the two photon decay channel is reported, using $1.08 \mathrm{fb}^{-1}$ of proton-proton collision data at a centre-of-mass energy of 7 TeV recorded by the ATLAS detector. No significant excess is observed in the investigated mass range of $110-150 \mathrm{GeV}$. Upper limits on the cross-section times branching ratio of between 2.0 and 5.8 times the Standard Model prediction are derived for this mass range.


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## 1. Introduction

The search for the Standard Model Higgs boson [1-3] is one of the key goals of the Large Hadron Collider (LHC) at CERN. The allowed Higgs boson mass ( $m_{H}$ ) is constrained at the $95 \%$ confidence level by a lower limit of 114.4 GeV from the LEP experiments [4] and an excluded region between 156 and 177 GeV from the Tevatron experiments [5,6]. First results have been reported by the ATLAS experiment in a variety of channels [7] and the CMS experiment [8] using the data recorded in 2010, which correspond to an integrated luminosity about thirty times smaller than the 2011 dataset used in this analysis.

In the low mass range, from the LEP limit to $m_{H} \approx 140 \mathrm{GeV}$, one of the most promising search channels at the LHC is the rare decay of the Higgs boson into a pair of photons. Despite the low branching ratio ( $\approx 0.2 \%$ ), this channel provides good experimental sensitivity in the mass region below 150 GeV . The results presented in this Letter are based on proton-proton collision data taken at $\sqrt{s}=7 \mathrm{TeV}$ by the ATLAS experiment between April and June 2011.

The data analysis proceeds by selecting photon pairs with tight identification and isolation cuts to minimize backgrounds other than direct diphoton production. A narrow peak in the reconstructed invariant mass distribution is searched for over a large, smooth background whose normalisation and shape are left free in a maximum likelihood fit. To increase the sensitivity, the sample is divided into five categories based on the presence of photon conversions and on the photon impact point on the calorimeter, with different invariant mass resolutions and signal-to-background ratios for the different categories.

[^0]The results of the fit are compared to the prediction from the Standard Model using the Higgs boson production cross-section and branching ratio from Ref. [9]. Limits on the production crosssection relative to the Standard Model value are then derived as a function of the hypothesised Higgs boson mass. Although with the current dataset the analysis is not yet sensitive to the predicted rate for a Standard Model Higgs boson, the limits on the yield in this decay channel improve on those obtained in the same channel by the Tevatron experiments [10-12], and are sensitive to possible enhancements in the Higgs boson production and decay rate compared with the Standard Model expectations.

## 2. Experimental setup and data set

The ATLAS detector is described in detail in Ref. [13]. The main subdetectors relevant to this analysis are the calorimeter, in particular its electromagnetic section, and the inner tracking detector.

The electromagnetic calorimeter is a lead-liquid argon sampling calorimeter with accordion geometry. It is divided into a barrel section covering the pseudorapidity ${ }^{1}$ region $|\eta|<1.45$ and two end-cap sections covering the pseudorapidity region $1.375<|\eta|<$ 3.2. It has three longitudinal layers. The first one, with a thickness between 3 and 5 radiation lengths, has a high granularity in $\eta$ (between 0.003 and 0.006 depending on $\eta$, with the exception of the regions $1.4<|\eta|<1.5$ and $|\eta|>2.4$ ), sufficient to provide discrimination between single photon showers and two photons from a $\pi^{0}$ decay. The second layer has a thickness of around 17 radiation lengths and a granularity of $0.025 \times 0.025$ in $\eta \times \phi$.

[^1]A third layer, with a thickness varying between 4 and 15 radiation lengths, is used to correct for leakage beyond the calorimeter for high energy showers. In front of the calorimeter, a thin presampler layer, covering $|\eta|<1.8$, is used to correct for fluctuations in upstream energy losses. The sampling term $a$ of the energy resolution, $\sigma(E) / E \approx a / \sqrt{E(\mathrm{GeV})}$, varies between $9 \%$ and $14 \%$ as a function of $|\eta|$ for unconverted photons [14]. It reaches up to $20 \%$ for converted photons near $|\eta|$ of 1.3 where the upstream material effect is the largest. The sampling term is the largest contribution to the resolution up to about 100 GeV , where the constant term starts to dominate. After $0.17 \mathrm{fb}^{-1}$ of data were accumulated, some calorimeter cells could not be read out. The affected region size is $\Delta \eta \times \Delta \phi \approx 1.5 \times 0.2$ in the barrel electromagnetic calorimeter, resulting in an acceptance loss for diphoton candidates of about $3 \%$. A hadronic sampling calorimeter is located behind the electromagnetic calorimeter. It is made of steel and scintillating tiles in the barrel section, and of copper and liquid argon in the end-cap.

The inner detector consists of three subsystems: at small radial distance $R$ from the beam axis ( $5<R<15 \mathrm{~cm}$ ), pixel silicon detectors are arranged in three cylindrical layers in the barrel and in three disks in each end-cap; at intermediate radii ( $30<R<$ 56 cm ), double layers of single-sided silicon microstrip detectors are used, organised in four cylindrical layers in the barrel and nine disks in each end-cap; at larger radii ( $56<R<107 \mathrm{~cm}$ ), a straw tracker with transition radiation capabilities is used. These three systems are immersed in a 2 T axial magnetic field. The silicon pixel and strip subsystems cover the range $|\eta|<2.5$, while the transition radiation tracker acceptance is limited to the range $|\eta|<2.0$. The inner detector allows reconstruction of secondary vertices, in particular of photon conversions occurring in the inner detector material up to a radius of $\approx 80 \mathrm{~cm}$.

The total amount of material in front of the first active layer of the electromagnetic calorimeter (including that in the presampler) varies between 2.5 and 6 radiation lengths as a function of pseudorapidity, excluding the transition region ( $1.37<|\eta|<1.52$ ) between the barrel and the end-caps.

Data used in this analysis were selected using a di-photon trigger with a 20 GeV transverse energy threshold on each photon. At the first trigger level, which uses reduced granularity, two clusters with transverse energies above 14 GeV are required in the electromagnetic calorimeter. At the higher trigger levels, loose photon identification cuts are applied using the full calorimeter granularity. This trigger has an efficiency greater than $99 \%$ for the signal after the final event selection.

In these data, the instantaneous luminosity varies between $\approx 10^{32} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ and $\approx 10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ with a bunch spacing of 50 ns. The average number of collisions per bunch crossing is around 6. Collisions in the same bunch crossing as the signal (in-time pileup) or in other bunch crossings within the detector sensitive time (out-of-time pileup) influence the event reconstruction. The inner detector is only sensitive to in-time pileup while the electromagnetic calorimeter is sensitive to pileup within a $\approx 450$ ns time window.

The application of beam, detector, and data-quality requirements to the recorded data results in a data sample corresponding to a total integrated luminosity of $(1.08 \pm 0.04) \mathrm{fb}^{-1}$ [15].

## 3. Simulated samples

The Higgs boson signal from the dominant gluon fusion production process (corresponding to $86 \%$ of the production crosssection for a Higgs boson with a mass of 120 GeV ) is generated with POWHEG [16]. MC@NLO [17] is used as a cross-check. POWHEG [18] is also used to generate the signal events from the
sub-leading vector boson fusion process ( $7 \%$ of the cross-section at 120 GeV ). For the other production modes, namely associated production with a $W$ or $Z$ boson or a $t \bar{t}$ pair, PYTHIA [19] is used.

The predicted signal is normalised using NNLO cross-sections for the gluon fusion process [20-24], the vector boson fusion process [25], the associated production with a $W$ or $Z$ boson [26] and NLO cross-section for the associated production with a $t \bar{t}$ pair [27]. The NLO electroweak corrections are applied to the gluon fusion [28,29], vector boson fusion [30,31], and the associated production with a $W$ or $Z$ boson [32] processes. The uncertainty on the theoretical cross-section is estimated [9] to be ${ }_{-15}^{+20} \%$, mostly due to the renormalisation and factorisation scale variations and the uncertainties in the parton distribution functions [33-36]. The Higgs boson decay branching fractions are taken from Refs. [9,37]. The uncertainty on the branching ratio to two photons is negligible compared with the cross-section uncertainty.

Signal events are generated in steps of 5 GeV for Higgs boson masses in the range of $110-150 \mathrm{GeV}$. PYTHIA and ALPGEN [38] have been chosen to generate the background samples, which are, however, only used for cross-checks and not to extract the final results.

All Monte Carlo (MC) samples are processed through a complete simulation of the ATLAS detector [39] using the GEANT4 programme [40]. Pileup effects are simulated by overlaying each MC event with a variable number of MC inelastic $p p$ collisions, taking into account both in-time and out-of-time pileup and the LHC bunch train structure. MC events are weighted to have the same distribution of average number of interactions per bunch crossing as in the data.

## 4. Photon reconstruction, event selection and backgrounds

### 4.1. Photon reconstruction

Photon reconstruction is seeded by energy clusters in the electromagnetic calorimeter with transverse energies exceeding 2.5 GeV in projective towers of size $0.075 \times 0.125$ in $\eta \times \phi$ made from the presampler and the three electromagnetic calorimeter layers. These energy clusters are then matched to tracks that are reconstructed in the inner detector and extrapolated to the calorimeter. Clusters without matching tracks are classified as unconverted photon candidates. Clusters matched to either pairs of tracks which are consistent with the hypothesis of a photon conversion or single tracks without hits in the pixel layer nearest to the beam pipe are considered as converted photon candidates. The photon reconstruction efficiency is $\approx 98 \%$.

The energy measurement is made in the electromagnetic calorimeter using a cluster size which depends on the photon classification. In the barrel, a size of $0.075 \times 0.125$ in $\eta \times \phi$ is used for unconverted photons and $0.075 \times 0.175$ for converted photon candidates, to account for the larger spread of the shower in $\phi$ for converted photons due to the magnetic field. In the end-cap, a cluster size of $0.125 \times 0.125$ is used for all candidates. A dedicated energy calibration [14] is applied to account for upstream energy losses, lateral leakage and longitudinal leakage, separately for converted and unconverted photon candidates.

The final energy calibration is determined from $Z \rightarrow e e$ decays, resulting in $\eta$-dependent correction factors of the order of $\pm 1 \%$. After this calibration procedure, the constant term in the energy resolution is estimated to be $1.1_{-0.6}^{+0.5} \%$ in the barrel region and $1.8_{-0.6}^{+0.5} \%$ in the end-cap region [41]. The energy resolution in the simulation is adjusted to match these values.

Photon identification is based on the lateral and longitudinal energy profiles of the shower in the calorimeter [42]. The photon candidate is required to deposit only a small fraction of its en-
ergy in the hadronic calorimeter. The transverse shower shape in the second layer of the electromagnetic calorimeter needs to be consistent with that expected for a single electromagnetic shower. Finally, the high granularity first layer is used to discriminate single photons from overlapping photon pairs from neutral meson decays produced in jet fragmentation, which are the main background source. Based on these criteria, a set of tight identification cuts, different for converted and unconverted candidates, is applied.

To take into account small differences in shower shapes between data and simulation, the shape variables are shifted in the simulation before the identification cuts are applied. The photon identification efficiency ranges typically from $75 \%$ to $90 \%$ for transverse energies between 25 and 100 GeV .

To increase the background rejection, an isolation cut is applied. The isolation variable [42] is computed by summing the transverse energy in calorimeter cells in a cone of radius 0.4 in the $\eta \times \phi$ space around the photon candidate. Cells in the electromagnetic calorimeter within $0.125 \times 0.175$ from the shower barycentre are excluded from the sum. The small photon energy leakage outside the excluded cells is evaluated as a function of the transverse energy in simulated samples and is subtracted from the isolation variable. To reduce the effect from the underlying event and pileup, the isolation is further corrected using a method suggested in Ref. [43]: for each of the two different pseudorapidity regions $|\eta|<1.5$ and $1.5<|\eta|<3.0$, low energy jets are used to compute an "ambient" energy density, which is then multiplied by the area of the isolation cone and subtracted from the isolation energy.

In the following, photon candidates having isolation transverse energies lower than 5 GeV are considered as isolated. The isolation cut efficiency is checked in data using a control sample of $Z \rightarrow e e$ events. The per-event efficiency of requiring both electrons to be isolated is found to be $3 \%$ lower in the data than in the simulated samples. In the MC, the isolation cut efficiency is found to be the same for $Z \rightarrow e e$ and $H \rightarrow \gamma \gamma$ events ( $\approx 93 \%$ ). The number of events predicted by the simulation after the isolation cut is therefore reduced by $3 \%$.

### 4.2. Event selection

Two photon candidates are required to pass tight identification criteria, to be isolated, and to be within the region $|\eta|<2.37$, excluding $1.37<|\eta|<1.52$, where the first calorimeter layer has high granularity. The highest and second highest photon transverse energies are required be above 40 and 25 GeV respectively. Both photons must be clear of problematic regions in the calorimeter. As the goal is to investigate Higgs boson mass hypotheses between 110 and 150 GeV , the invariant mass of the photon pair is required to be within $100-160 \mathrm{GeV}$. After these cuts 5063 events remain in the selected data sample.

The acceptance of the kinematic cuts, as estimated with generated photons in the MC signal samples, is $60 \%$ for the dominant gluon fusion process for a mass of 120 GeV . The overall event selection efficiency, taking into account both kinematic cut acceptance and reconstruction and identification efficiencies, is $39 \%$. The event selection efficiency is slightly larger in the vector boson fusion process. It is somewhat smaller in the associated production mode. It increases with the Higgs boson mass from $34 \%$ at 110 GeV to $43 \%$ at 150 GeV .

To enhance the sensitivity of the analysis, the data sample is split in five categories, with different invariant mass resolutions and different signal-to-background ratios:

- Unconverted central ( $8 \%$ of the candidates): Both photons are unconverted and in the central part of the barrel calorimeter

Table 1
Cross-section times branching ratio and expected numbers of signal events after all cuts (total and per category), for various Higgs boson masses and for an integrated luminosity of $1.08 \mathrm{fb}^{-1}$.

| $m_{H}[\mathrm{GeV}]$ | 110 | 120 | 130 | 140 | 150 |
| :--- | ---: | ---: | ---: | ---: | :---: |
| $\sigma \times$ BR [fb] | 45 | 43 | 37 | 27 | 16 |
| Signal yield | 17.0 | 17.6 | 15.8 | 12.1 | 7.7 |
| Unconverted central | 2.6 | 2.6 | 2.3 | 1.7 | 1.1 |
| Unconverted rest | 4.6 | 4.7 | 4.2 | 3.4 | 2.1 |
| Converted central | 2.0 | 2.0 | 1.7 | 1.3 | 0.8 |
| Converted transition | 2.3 | 2.2 | 2.1 | 1.5 | 1.0 |
| Converted rest | 5.6 | 6.0 | 5.6 | 4.2 | 2.7 |

( $|\eta|<0.75$ ). This is the category with the best invariant mass resolution and the best signal-to-background ratio;

- Unconverted rest ( $28 \%$ of the candidates): Both photons are unconverted and at least one photon does not lie in the central part of the barrel calorimeter;
- Converted central ( $7 \%$ of the candidates): At least one photon is converted and both photons are in the central part of the barrel calorimeter;
- Converted transition ( $16 \%$ of the candidates): At least one photon is converted and at least one photon is near the transition between barrel and end-cap calorimeter ( $1.3<|\eta|<1.75$ ). Given the larger amount of material in this region, the energy resolution, in particular for converted photons, can be significantly degraded;
- Converted rest ( $41 \%$ of the candidates): All other events with at least one converted photon.

Table 1 shows the cross-section times branching ratio to two photons, the expected total and per category signal yields for $1.08 \mathrm{fb}^{-1}$ for different Standard Model Higgs boson mass hypotheses. Using these categories improves the signal sensitivity of the analysis by around $15 \%$ for a 120 GeV Higgs boson mass compared with a fully inclusive analysis.

### 4.3. Invariant mass reconstruction

In addition to the energies, the angle between the photons is needed for the computation of the diphoton invariant mass. This angle is determined from the interaction vertex position and the photon impact points in the calorimeter. The resolution of the angle measurement is dominated by the reconstruction of the primary vertex $z$ position. The RMS vertex spread in the $z$ direction is $\approx 5.5 \mathrm{~cm}$, and a more accurate event-by-event estimate is performed to reduce the impact on the invariant mass resolution. Given the non-negligible level of pileup in the 2011 data, the determination of the vertex position is based only on the photon candidates, without relying on other charged tracks in the event. For converted photons with tracks having a precise measurement in the $z$ direction, the vertex position is estimated from the intercept of the line joining the reconstructed conversion position and the calorimeter impact point with the beam line. For all other photons, the vertex position is estimated from the shower position measurements in the first and second layers of the electromagnetic calorimeter, which can be used to calculate the photon direction. Finally, the vertex positions from both photons are combined taking also into account the average beam spot position in $z$. When both photons are unconverted, the typical vertex position resolution is $\approx 1.6 \mathrm{~cm}$ in $z$. The resolution is better in events with converted photons. The resulting impact of the angle measurement on the invariant mass resolution is negligible compared to the contribution from the photon energy resolution.


Fig. 1. Distribution of the reconstructed diphoton invariant mass of a simulated 120 GeV mass Higgs boson signal, for all categories together. The line shows the fit of the mass resolution using the function described in the text. The core component of the mass resolution is 1.7 GeV .

Fig. 1 shows the invariant mass distribution for simulated Higgs boson events with mass 120 GeV . The mass resolution for the signal is modelled by the sum of a Crystal Ball function [44] (for the bulk of the events which have a narrow Gaussian spectrum in the peak region and tails toward lower reconstructed mass) and a Gaussian distribution with a wide sigma (to model the far outliers in the distribution). The Crystal Ball function is defined as:
$N \cdot \begin{cases}e^{-t^{2} / 2} & \text { if } t>-\alpha_{C B}, \\ \left(\frac{n_{C B}}{\alpha_{C B}}\right)^{n_{C B}} \cdot e^{-\alpha_{C B}^{2} / 2} \cdot\left(\frac{n_{C B}}{\alpha_{C B}}-\alpha_{C B}-t\right)^{-n_{C B}} & \text { otherwise }\end{cases}$
where $t=\left(m_{\gamma \gamma}-\mu_{C B}\right) / \sigma_{C B}, N$ is a normalisation parameter, $\mu_{C B}$ is the peak of the narrow Gaussian distribution, $\sigma_{C B}$ represents the Gaussian resolution for the core component, and $n_{C B}$ and $\alpha_{C B}$ parametrise the non-Gaussian tail.

The core component of the mass resolution, $\sigma_{C B}$, ranges from 1.4 GeV in the "Unconverted central" category to 2.1 GeV in the "Converted transition" category. The non-Gaussian contributions to the mass resolution arise mostly from converted photons with at least one electron losing a significant fraction of its energy through bremsstrahlung in the inner detector material.

### 4.4. Sample composition

The main background components are the diphoton production, the photon-jet production with one fake photon from jets fragmenting into a high energy $\pi^{0}$, the dijet production with two fake photons, and Drell-Yan events where both electrons are misidentified as photons. A measurement of the diphoton production crosssection with 2010 ATLAS data can be found in Ref. [45], where the techniques used to estimate the purity of the sample are described in more detail. Although the final result does not rely on it, a quantitative understanding of the sample composition is an important cross-check of the diphoton selection procedure.

A method based on the use of control regions for two discriminating variables is applied to measure the contributions of fake photon background directly from the data. This method exploits relaxed isolation and photon identification cuts to estimate the fake components, by relying on the fact that the rejections from these two cuts are almost independent. It is a generalisation of the method used in Ref. [42]. The Drell-Yan background is estimated by measuring the probability for an electron to be reconstructed as a photon candidate with $Z$ events and applying this probability to the observed yield of Drell-Yan events at high mass.

The number of diphoton events in the $100-160 \mathrm{GeV}$ mass range is found to be $3650 \pm 100 \pm 290$, where the first uncertainty is sta-


Fig. 2. Diphoton, photon-jet, dijet and Drell-Yan contributions to the diphoton candidate invariant mass distribution, as obtained from a data-driven method. The various components are stacked on top of each other. The error bars correspond to the uncertainties on each component separately.
tistical and the second is systematic. The systematic uncertainty arises from the definition of the relaxed identification control region, the possible correlations between isolation and identification variables, and the fraction of real photons leaking into the background control regions. The extracted yields of photon-jet and dijet are $1110 \pm 60 \pm 270$ and $220 \pm 20 \pm 130$ events respectively. The Drell-Yan background, which is most prominent in the categories with at least one converted photon, is estimated to be $86 \pm 1 \pm 14$ events in the mass range of $100-160 \mathrm{GeV}$.

Fig. 2 shows the extracted components of the diphoton, photonjet, dijet and Drell-Yan processes. The purity of the sample (fraction of diphoton events) is about $72 \%$. The measurement of the purity has also been made separately in each category, and ranges from $69 \%$ to $83 \%$.

Other methods have been used to cross-check the purity estimate, in particular using template fits of the photon isolation distribution, where both signal and background templates are derived from data. The results are in agreement with the results quoted here.

## 5. Systematic uncertainties

Experimental systematic uncertainties affecting the extraction of the signal from the diphoton invariant mass distribution related to the modelling of the signal can be classified in two types: uncertainties affecting the predicted yield and uncertainties affecting the modelling of the mass resolution.

The uncertainties on the event yield are the following:

- The uncertainty from the photon reconstruction and identification efficiency amounts to $\pm 11 \%$ per event. It is estimated from data and MC differences in shower shape variables, the impact of additional material in front of the calorimeter and the impact of pileup on the photon shower shape variables.
- The uncertainty on the isolation cut efficiency is taken as the difference between data and MC found in $Z \rightarrow e e$ decays and amounts to $\pm 3 \%$ per event.
- The uncertainty on the photon trigger efficiency is $\pm 1 \%$. It comes from the uncertainty in the measurement of the trigger efficiency for diphoton candidates using control triggers and from possible differences between the trigger efficiency for photons from Higgs boson decays and all diphoton candidates.
- The uncertainty on the kinematic cut acceptance from the modelling of the Higgs boson transverse momentum distribu-
tion is investigated with HQT [46] and RESBOS [47,48], which account for all-orders soft-gluon resummation up to NNLL accuracy. The resulting uncertainty is found to be at the level of $\pm 1 \%$.
- The luminosity uncertainty is $3.7 \%$ [15].

The total uncertainty on the expected signal event yield is $\pm 12 \%$.
The uncertainties on the invariant mass resolution are the following:

- The uncertainty on the cluster energy resolution comes from the uncertainty on the sampling term, estimated to be $10 \%$, and from the uncertainty on the constant term, which is estimated using $Z \rightarrow$ ee decays. Both uncertainties are taken into account with their proper correlation from the Z control sample constraint. The uncertainty on the cluster energy resolution amounts to a $\pm 12 \%$ relative uncertainty on the diphoton invariant mass resolution.
- The uncertainty on the photon energy calibration arising from the extrapolation of the electron energy scale calibration is estimated from MC studies. The difference between the photon and the electron response in the calorimeter comes from the material in front of the active part of the calorimeter. The uncertainty is estimated using simulations with a different amount of material in front of the calorimeter and is found to be $\pm 6 \%$ on the mass resolution.
- The contribution of pileup fluctuations to the cluster energy measurement is checked using random clusters in randomly triggered bunch crossings, with a frequency corresponding to expectations from the instantaneous luminosity. The relative uncertainty on the mass resolution is found to be less than $3 \%$.
- The uncertainty on the resolution of the photon angle measurement is studied with $Z \rightarrow$ ee decays. The calorimeterbased direction measurement is compared with the much more precise track-based direction measurement. In the barrel calorimeter, the resolution measured in data agrees well with the one predicted by the simulation. In the end-cap region, the resolution measured in data is $\approx 20 \%$ worse than in the simulation. The impact of this difference is a $1 \%$ relative uncertainty on the diphoton mass resolution.

The total relative uncertainty on the diphoton invariant mass resolution is thus $\pm 14 \%$. This systematic uncertainty is applied to both the Crystal Ball and the wide Gaussian resolution parameters.

These systematic uncertainties are taken as fully correlated between the different categories. The impact of uncorrelated systematic uncertainties in the different categories and migration between categories has been investigated and found to be negligible.

The background is modelled by an exponentially falling invariant mass distribution. Systematic uncertainties arise from possible deviations of the background distribution from this assumed shape. This has been estimated by checking how accurately the chosen model fits different predicted diphoton mass distributions [49, 50] and comparing different functional forms for the background model. The resulting uncertainty is between $\pm 5$ events at 110 GeV and $\pm 3$ events at 150 GeV for a Higgs boson mass signal region about 4 GeV wide.

## 6. Results

The data are compared to background and signal-plus-background hypotheses using a profile likelihood test statistic as described in Refs. [7,51]. The exponentially falling invariant mass distribution used for the background model is determined by two

## Table 2

Fractions of background $\left(f_{b}\right)$, predicted signal $\left(f_{s}\right)$ and core Gaussian mass resolution $(\sigma)$ in each category for a Higgs boson mass hypothesis of 120 GeV . The fractions are normalised to the total yield summed over categories.

| Category | $f_{b}$ | $f_{s}$ | $\sigma(\mathrm{GeV})$ |
| :--- | ---: | :--- | :--- |
| Unconverted central | $7 \%$ | $15 \%$ | 1.4 |
| Unconverted rest | $29 \%$ | $27 \%$ | 1.6 |
| Converted central | $8 \%$ | $11 \%$ | 1.5 |
| Converted transition | $16 \%$ | $13 \%$ | 2.1 |
| Converted rest | $40 \%$ | $34 \%$ | 1.8 |



Fig. 3. Distribution of the reconstructed diphoton mass. All five diphoton categories have been combined. The exponential fit to the full sample of the background-only hypothesis, as well as the expected signal for a Higgs boson mass of 120 GeV with five times the Standard Model predicted yield, are also shown for illustration.
nuisance parameters per category (the normalisation and the exponential negative slope), which are left free in the unbinned fit. The signal is modelled with the mass resolution functions described above, one per category, fixing the fraction of events in each category to the MC predictions. Table 2 summarises the measured fractions of background events in each category, the predicted fractions of signal events and the predicted core Gaussian signal mass resolutions for a Higgs boson mass hypothesis of 120 GeV .

The fitted parameters for the signal are thus the overall signal strength relative to the Standard Model prediction and the nuisance parameters on the predicted event yield and mass resolution which have Gaussian constraints in the fit. The uncertainty on the predicted event yield includes both the experimental systematic uncertainties described in Section 5 and the uncertainty on the predicted cross-section described in Section 3. The systematic uncertainty on the background shape is included as another nuisance parameter with a Gaussian constraint in the fit. From this fit, the best estimate of the signal yield is extracted, as well as the likelihood ratio (profile likelihood) between any assumed signal yield (leaving the nuisance parameters free to maximise the likelihood) and the best estimate. The fit is performed in 1 GeV steps for the Higgs boson mass hypothesis, which is significantly smaller than the invariant mass resolution. The signal parameters for these fine mass steps are interpolated from the fully simulated samples.

Fig. 3 shows the reconstructed diphoton mass spectrum. No excess is visible. This is quantified by the $p$-value of the backgroundonly hypothesis, which gives the fraction of background-only experiments that would have a profile likelihood ratio of the zero signal hypothesis relative to the best-fitted signal strength at least as low as the one found in the data. Negative signals are not allowed in the fit, so $p$-values above 0.5 are truncated. This $p$-value is shown in Fig. 4(a) as a function of the hypothesised Higgs boson mass. The minimal $p$-value, corresponding to the largest back-


Fig. 4. (a) $p$-value ( $p_{0}$ ) of the background-only hypothesis as a function of the investigated Higgs boson mass; (b) $95 \%$ confidence level upper limits on a Standard Model Higgs boson production cross-section, relative to the Standard Model crosssection, as a function of Higgs boson mass hypothesis. The solid line shows the observed limit. The dashed line shows the median expected limit for background-only pseudo-experiments, with the bands indicating the expected fluctuations around this limit at the $1 \sigma$ and $2 \sigma$ levels.
ground upward fluctuation, is $\approx 5 \%$ and is found for a hypothesised mass of $\approx 128 \mathrm{GeV}$. The probability for such an excess to appear anywhere in the investigated mass range is around $40 \%$.

Exclusion limits on the inclusive production cross-section of a Standard Model Higgs boson relative to the Standard Model crosssection are derived. For this purpose, a modified frequentist approach $C L_{s}$ [52], corresponding to the ratio of $p$-values for the signal-plus-background and the background-only hypothesis for a given assumed signal strength is used. A given signal strength is excluded at $95 \%$ confidence level if its $C L_{s}$ is smaller than 0.05 . The confidence levels are computed using a large number of signal-plus-background pseudo-experiments, with different signal yields, and background-only pseudo-experiments. The results, including systematic uncertainties, are shown in Fig. 4(b). The impact of the experimental systematic uncertainties is about $5 \%$ on the expected limit for the mass hypothesis of 120 GeV .

The expected median limit in the case of no signal varies from 3.3 to 5.8 as a function of the Higgs boson mass. The variations of the observed limit, between 2.0 and 5.8 , are consistent with expected statistical fluctuations around the median limit.

## 7. Conclusions

A search for the Standard Model Higgs boson in the $H \rightarrow \gamma \gamma$ decay mode has been performed using an integrated luminosity of $1.08 \mathrm{fb}^{-1}$ recorded by the ATLAS experiment in 2011. A high purity diphoton sample is selected. No excess is found in the diphoton invariant mass distribution in the mass range of $110-150 \mathrm{GeV}$. The observed limit on the cross-section of a Standard Model-like Higgs
boson decaying into a pair of photons ranges between 2.0 and 5.8 times the Standard Model cross-section. These variations are compatible with statistical fluctuations around the expected limit for this data set. These limits are the most stringent to date in this channel.

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Grybel ${ }^{141}$, V.J. Guarino ${ }^{5}$, D. Guest ${ }^{175}$, C. Guicheney ${ }^{33}$, A. Guida ${ }^{72 \mathrm{a}, 72 \mathrm{~b}}$, T. Guillemin ${ }^{4}$, S. Guindon ${ }^{54}$, H. Guler ${ }^{85, n}$, J. Gunther ${ }^{125}$, B. Guo ${ }^{158}$, J. Guo ${ }^{34}$, A. Gupta ${ }^{30}$, Y. Gusakov ${ }^{65}$, V.N. Gushchin ${ }^{128}$, A. Gutierrez ${ }^{93}$, P. Gutierrez ${ }^{111}$, N. Guttman ${ }^{153}$, O. Gutzwiller ${ }^{172}$, C. Guyot ${ }^{136}$, C. Gwenlan ${ }^{118}$, C.B. Gwilliam ${ }^{73}$, A. Haas ${ }^{143}$, S. Haas ${ }^{29}$, C. Haber ${ }^{14}$, R. Hackenburg ${ }^{24}$, H.K. Hadavand ${ }^{39}$, D.R. Hadley ${ }^{17}$, P. Haefner ${ }^{99}$, F. Hahn ${ }^{29}$, S. Haider ${ }^{29}$, Z. Hajduk ${ }^{38}$, H. Hakobyan ${ }^{176}$, J. Haller ${ }^{54}$, K. Hamacher ${ }^{174}$, P. Hamal ${ }^{113}$, A. Hamilton ${ }^{49}$, S. Hamilton ${ }^{161}$, H. Han ${ }^{32 a}$, L. Han ${ }^{32 b}$, K. Hanagaki ${ }^{116}$, M. Hance ${ }^{120}$, C. Handel ${ }^{81}$, P. 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# Search for the Standard Model Higgs boson in the two photon decay channel with the ATLAS detector at the LHC ${ }^{\text {N }}$ 

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#### Abstract

A search for the Standard Model Higgs boson in the two photon decay channel is reported, using $1.08 \mathrm{fb}^{-1}$ of proton-proton collision data at a centre-of-mass energy of 7 TeV recorded by the ATLAS detector. No significant excess is observed in the investigated mass range of $110-150 \mathrm{GeV}$. Upper limits on the cross-section times branching ratio of between 2.0 and 5.8 times the Standard Model prediction are derived for this mass range.


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## 1. Introduction

The search for the Standard Model Higgs boson [1-3] is one of the key goals of the Large Hadron Collider (LHC) at CERN. The allowed Higgs boson mass ( $m_{H}$ ) is constrained at the $95 \%$ confidence level by a lower limit of 114.4 GeV from the LEP experiments [4] and an excluded region between 156 and 177 GeV from the Tevatron experiments [5,6]. First results have been reported by the ATLAS experiment in a variety of channels [7] and the CMS experiment [8] using the data recorded in 2010, which correspond to an integrated luminosity about thirty times smaller than the 2011 dataset used in this analysis.

In the low mass range, from the LEP limit to $m_{H} \approx 140 \mathrm{GeV}$, one of the most promising search channels at the LHC is the rare decay of the Higgs boson into a pair of photons. Despite the low branching ratio ( $\approx 0.2 \%$ ), this channel provides good experimental sensitivity in the mass region below 150 GeV . The results presented in this Letter are based on proton-proton collision data taken at $\sqrt{s}=7 \mathrm{TeV}$ by the ATLAS experiment between April and June 2011.

The data analysis proceeds by selecting photon pairs with tight identification and isolation cuts to minimize backgrounds other than direct diphoton production. A narrow peak in the reconstructed invariant mass distribution is searched for over a large, smooth background whose normalisation and shape are left free in a maximum likelihood fit. To increase the sensitivity, the sample is divided into five categories based on the presence of photon conversions and on the photon impact point on the calorimeter, with different invariant mass resolutions and signal-to-background ratios for the different categories.

[^3]The results of the fit are compared to the prediction from the Standard Model using the Higgs boson production cross-section and branching ratio from Ref. [9]. Limits on the production crosssection relative to the Standard Model value are then derived as a function of the hypothesised Higgs boson mass. Although with the current dataset the analysis is not yet sensitive to the predicted rate for a Standard Model Higgs boson, the limits on the yield in this decay channel improve on those obtained in the same channel by the Tevatron experiments [10-12], and are sensitive to possible enhancements in the Higgs boson production and decay rate compared with the Standard Model expectations.

## 2. Experimental setup and data set

The ATLAS detector is described in detail in Ref. [13]. The main subdetectors relevant to this analysis are the calorimeter, in particular its electromagnetic section, and the inner tracking detector.

The electromagnetic calorimeter is a lead-liquid argon sampling calorimeter with accordion geometry. It is divided into a barrel section covering the pseudorapidity ${ }^{1}$ region $|\eta|<1.45$ and two end-cap sections covering the pseudorapidity region $1.375<|\eta|<$ 3.2. It has three longitudinal layers. The first one, with a thickness between 3 and 5 radiation lengths, has a high granularity in $\eta$ (between 0.003 and 0.006 depending on $\eta$, with the exception of the regions $1.4<|\eta|<1.5$ and $|\eta|>2.4$ ), sufficient to provide discrimination between single photon showers and two photons from a $\pi^{0}$ decay. The second layer has a thickness of around 17 radiation lengths and a granularity of $0.025 \times 0.025$ in $\eta \times \phi$.

[^4]A third layer, with a thickness varying between 4 and 15 radiation lengths, is used to correct for leakage beyond the calorimeter for high energy showers. In front of the calorimeter, a thin presampler layer, covering $|\eta|<1.8$, is used to correct for fluctuations in upstream energy losses. The sampling term $a$ of the energy resolution, $\sigma(E) / E \approx a / \sqrt{E(\mathrm{GeV})}$, varies between $9 \%$ and $14 \%$ as a function of $|\eta|$ for unconverted photons [14]. It reaches up to $20 \%$ for converted photons near $|\eta|$ of 1.3 where the upstream material effect is the largest. The sampling term is the largest contribution to the resolution up to about 100 GeV , where the constant term starts to dominate. After $0.17 \mathrm{fb}^{-1}$ of data were accumulated, some calorimeter cells could not be read out. The affected region size is $\Delta \eta \times \Delta \phi \approx 1.5 \times 0.2$ in the barrel electromagnetic calorimeter, resulting in an acceptance loss for diphoton candidates of about $3 \%$. A hadronic sampling calorimeter is located behind the electromagnetic calorimeter. It is made of steel and scintillating tiles in the barrel section, and of copper and liquid argon in the end-cap.

The inner detector consists of three subsystems: at small radial distance $R$ from the beam axis ( $5<R<15 \mathrm{~cm}$ ), pixel silicon detectors are arranged in three cylindrical layers in the barrel and in three disks in each end-cap; at intermediate radii ( $30<R<$ 56 cm ), double layers of single-sided silicon microstrip detectors are used, organised in four cylindrical layers in the barrel and nine disks in each end-cap; at larger radii ( $56<R<107 \mathrm{~cm}$ ), a straw tracker with transition radiation capabilities is used. These three systems are immersed in a 2 T axial magnetic field. The silicon pixel and strip subsystems cover the range $|\eta|<2.5$, while the transition radiation tracker acceptance is limited to the range $|\eta|<2.0$. The inner detector allows reconstruction of secondary vertices, in particular of photon conversions occurring in the inner detector material up to a radius of $\approx 80 \mathrm{~cm}$.

The total amount of material in front of the first active layer of the electromagnetic calorimeter (including that in the presampler) varies between 2.5 and 6 radiation lengths as a function of pseudorapidity, excluding the transition region ( $1.37<|\eta|<1.52$ ) between the barrel and the end-caps.

Data used in this analysis were selected using a di-photon trigger with a 20 GeV transverse energy threshold on each photon. At the first trigger level, which uses reduced granularity, two clusters with transverse energies above 14 GeV are required in the electromagnetic calorimeter. At the higher trigger levels, loose photon identification cuts are applied using the full calorimeter granularity. This trigger has an efficiency greater than $99 \%$ for the signal after the final event selection.

In these data, the instantaneous luminosity varies between $\approx 10^{32} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ and $\approx 10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ with a bunch spacing of 50 ns. The average number of collisions per bunch crossing is around 6. Collisions in the same bunch crossing as the signal (in-time pileup) or in other bunch crossings within the detector sensitive time (out-of-time pileup) influence the event reconstruction. The inner detector is only sensitive to in-time pileup while the electromagnetic calorimeter is sensitive to pileup within a $\approx 450$ ns time window.

The application of beam, detector, and data-quality requirements to the recorded data results in a data sample corresponding to a total integrated luminosity of $(1.08 \pm 0.04) \mathrm{fb}^{-1}$ [15].

## 3. Simulated samples

The Higgs boson signal from the dominant gluon fusion production process (corresponding to $86 \%$ of the production crosssection for a Higgs boson with a mass of 120 GeV ) is generated with POWHEG [16]. MC@NLO [17] is used as a cross-check. POWHEG [18] is also used to generate the signal events from the
sub-leading vector boson fusion process ( $7 \%$ of the cross-section at 120 GeV ). For the other production modes, namely associated production with a $W$ or $Z$ boson or a $t \bar{t}$ pair, PYTHIA [19] is used.

The predicted signal is normalised using NNLO cross-sections for the gluon fusion process [20-24], the vector boson fusion process [25], the associated production with a $W$ or $Z$ boson [26] and NLO cross-section for the associated production with a $t \bar{t}$ pair [27]. The NLO electroweak corrections are applied to the gluon fusion [28,29], vector boson fusion [30,31], and the associated production with a $W$ or $Z$ boson [32] processes. The uncertainty on the theoretical cross-section is estimated [9] to be ${ }_{-15}^{+20} \%$, mostly due to the renormalisation and factorisation scale variations and the uncertainties in the parton distribution functions [33-36]. The Higgs boson decay branching fractions are taken from Refs. [9,37]. The uncertainty on the branching ratio to two photons is negligible compared with the cross-section uncertainty.

Signal events are generated in steps of 5 GeV for Higgs boson masses in the range of $110-150 \mathrm{GeV}$. PYTHIA and ALPGEN [38] have been chosen to generate the background samples, which are, however, only used for cross-checks and not to extract the final results.

All Monte Carlo (MC) samples are processed through a complete simulation of the ATLAS detector [39] using the GEANT4 programme [40]. Pileup effects are simulated by overlaying each MC event with a variable number of MC inelastic $p p$ collisions, taking into account both in-time and out-of-time pileup and the LHC bunch train structure. MC events are weighted to have the same distribution of average number of interactions per bunch crossing as in the data.

## 4. Photon reconstruction, event selection and backgrounds

### 4.1. Photon reconstruction

Photon reconstruction is seeded by energy clusters in the electromagnetic calorimeter with transverse energies exceeding 2.5 GeV in projective towers of size $0.075 \times 0.125$ in $\eta \times \phi$ made from the presampler and the three electromagnetic calorimeter layers. These energy clusters are then matched to tracks that are reconstructed in the inner detector and extrapolated to the calorimeter. Clusters without matching tracks are classified as unconverted photon candidates. Clusters matched to either pairs of tracks which are consistent with the hypothesis of a photon conversion or single tracks without hits in the pixel layer nearest to the beam pipe are considered as converted photon candidates. The photon reconstruction efficiency is $\approx 98 \%$.

The energy measurement is made in the electromagnetic calorimeter using a cluster size which depends on the photon classification. In the barrel, a size of $0.075 \times 0.125$ in $\eta \times \phi$ is used for unconverted photons and $0.075 \times 0.175$ for converted photon candidates, to account for the larger spread of the shower in $\phi$ for converted photons due to the magnetic field. In the end-cap, a cluster size of $0.125 \times 0.125$ is used for all candidates. A dedicated energy calibration [14] is applied to account for upstream energy losses, lateral leakage and longitudinal leakage, separately for converted and unconverted photon candidates.

The final energy calibration is determined from $Z \rightarrow e e$ decays, resulting in $\eta$-dependent correction factors of the order of $\pm 1 \%$. After this calibration procedure, the constant term in the energy resolution is estimated to be $1.1_{-0.6}^{+0.5} \%$ in the barrel region and $1.8_{-0.6}^{+0.5} \%$ in the end-cap region [41]. The energy resolution in the simulation is adjusted to match these values.

Photon identification is based on the lateral and longitudinal energy profiles of the shower in the calorimeter [42]. The photon candidate is required to deposit only a small fraction of its en-
ergy in the hadronic calorimeter. The transverse shower shape in the second layer of the electromagnetic calorimeter needs to be consistent with that expected for a single electromagnetic shower. Finally, the high granularity first layer is used to discriminate single photons from overlapping photon pairs from neutral meson decays produced in jet fragmentation, which are the main background source. Based on these criteria, a set of tight identification cuts, different for converted and unconverted candidates, is applied.

To take into account small differences in shower shapes between data and simulation, the shape variables are shifted in the simulation before the identification cuts are applied. The photon identification efficiency ranges typically from $75 \%$ to $90 \%$ for transverse energies between 25 and 100 GeV .

To increase the background rejection, an isolation cut is applied. The isolation variable [42] is computed by summing the transverse energy in calorimeter cells in a cone of radius 0.4 in the $\eta \times \phi$ space around the photon candidate. Cells in the electromagnetic calorimeter within $0.125 \times 0.175$ from the shower barycentre are excluded from the sum. The small photon energy leakage outside the excluded cells is evaluated as a function of the transverse energy in simulated samples and is subtracted from the isolation variable. To reduce the effect from the underlying event and pileup, the isolation is further corrected using a method suggested in Ref. [43]: for each of the two different pseudorapidity regions $|\eta|<1.5$ and $1.5<|\eta|<3.0$, low energy jets are used to compute an "ambient" energy density, which is then multiplied by the area of the isolation cone and subtracted from the isolation energy.

In the following, photon candidates having isolation transverse energies lower than 5 GeV are considered as isolated. The isolation cut efficiency is checked in data using a control sample of $Z \rightarrow e e$ events. The per-event efficiency of requiring both electrons to be isolated is found to be $3 \%$ lower in the data than in the simulated samples. In the MC, the isolation cut efficiency is found to be the same for $Z \rightarrow e e$ and $H \rightarrow \gamma \gamma$ events ( $\approx 93 \%$ ). The number of events predicted by the simulation after the isolation cut is therefore reduced by $3 \%$.

### 4.2. Event selection

Two photon candidates are required to pass tight identification criteria, to be isolated, and to be within the region $|\eta|<2.37$, excluding $1.37<|\eta|<1.52$, where the first calorimeter layer has high granularity. The highest and second highest photon transverse energies are required be above 40 and 25 GeV respectively. Both photons must be clear of problematic regions in the calorimeter. As the goal is to investigate Higgs boson mass hypotheses between 110 and 150 GeV , the invariant mass of the photon pair is required to be within $100-160 \mathrm{GeV}$. After these cuts 5063 events remain in the selected data sample.

The acceptance of the kinematic cuts, as estimated with generated photons in the MC signal samples, is $60 \%$ for the dominant gluon fusion process for a mass of 120 GeV . The overall event selection efficiency, taking into account both kinematic cut acceptance and reconstruction and identification efficiencies, is $39 \%$. The event selection efficiency is slightly larger in the vector boson fusion process. It is somewhat smaller in the associated production mode. It increases with the Higgs boson mass from $34 \%$ at 110 GeV to $43 \%$ at 150 GeV .

To enhance the sensitivity of the analysis, the data sample is split in five categories, with different invariant mass resolutions and different signal-to-background ratios:

- Unconverted central ( $8 \%$ of the candidates): Both photons are unconverted and in the central part of the barrel calorimeter

Table 1
Cross-section times branching ratio and expected numbers of signal events after all cuts (total and per category), for various Higgs boson masses and for an integrated luminosity of $1.08 \mathrm{fb}^{-1}$.

| $m_{H}[\mathrm{GeV}]$ | 110 | 120 | 130 | 140 | 150 |
| :--- | ---: | ---: | ---: | ---: | :---: |
| $\sigma \times$ BR [fb] | 45 | 43 | 37 | 27 | 16 |
| Signal yield | 17.0 | 17.6 | 15.8 | 12.1 | 7.7 |
| Unconverted central | 2.6 | 2.6 | 2.3 | 1.7 | 1.1 |
| Unconverted rest | 4.6 | 4.7 | 4.2 | 3.4 | 2.1 |
| Converted central | 2.0 | 2.0 | 1.7 | 1.3 | 0.8 |
| Converted transition | 2.3 | 2.2 | 2.1 | 1.5 | 1.0 |
| Converted rest | 5.6 | 6.0 | 5.6 | 4.2 | 2.7 |

( $|\eta|<0.75$ ). This is the category with the best invariant mass resolution and the best signal-to-background ratio;

- Unconverted rest ( $28 \%$ of the candidates): Both photons are unconverted and at least one photon does not lie in the central part of the barrel calorimeter;
- Converted central ( $7 \%$ of the candidates): At least one photon is converted and both photons are in the central part of the barrel calorimeter;
- Converted transition ( $16 \%$ of the candidates): At least one photon is converted and at least one photon is near the transition between barrel and end-cap calorimeter ( $1.3<|\eta|<1.75$ ). Given the larger amount of material in this region, the energy resolution, in particular for converted photons, can be significantly degraded;
- Converted rest ( $41 \%$ of the candidates): All other events with at least one converted photon.

Table 1 shows the cross-section times branching ratio to two photons, the expected total and per category signal yields for $1.08 \mathrm{fb}^{-1}$ for different Standard Model Higgs boson mass hypotheses. Using these categories improves the signal sensitivity of the analysis by around $15 \%$ for a 120 GeV Higgs boson mass compared with a fully inclusive analysis.

### 4.3. Invariant mass reconstruction

In addition to the energies, the angle between the photons is needed for the computation of the diphoton invariant mass. This angle is determined from the interaction vertex position and the photon impact points in the calorimeter. The resolution of the angle measurement is dominated by the reconstruction of the primary vertex $z$ position. The RMS vertex spread in the $z$ direction is $\approx 5.5 \mathrm{~cm}$, and a more accurate event-by-event estimate is performed to reduce the impact on the invariant mass resolution. Given the non-negligible level of pileup in the 2011 data, the determination of the vertex position is based only on the photon candidates, without relying on other charged tracks in the event. For converted photons with tracks having a precise measurement in the $z$ direction, the vertex position is estimated from the intercept of the line joining the reconstructed conversion position and the calorimeter impact point with the beam line. For all other photons, the vertex position is estimated from the shower position measurements in the first and second layers of the electromagnetic calorimeter, which can be used to calculate the photon direction. Finally, the vertex positions from both photons are combined taking also into account the average beam spot position in $z$. When both photons are unconverted, the typical vertex position resolution is $\approx 1.6 \mathrm{~cm}$ in $z$. The resolution is better in events with converted photons. The resulting impact of the angle measurement on the invariant mass resolution is negligible compared to the contribution from the photon energy resolution.


Fig. 1. Distribution of the reconstructed diphoton invariant mass of a simulated 120 GeV mass Higgs boson signal, for all categories together. The line shows the fit of the mass resolution using the function described in the text. The core component of the mass resolution is 1.7 GeV .

Fig. 1 shows the invariant mass distribution for simulated Higgs boson events with mass 120 GeV . The mass resolution for the signal is modelled by the sum of a Crystal Ball function [44] (for the bulk of the events which have a narrow Gaussian spectrum in the peak region and tails toward lower reconstructed mass) and a Gaussian distribution with a wide sigma (to model the far outliers in the distribution). The Crystal Ball function is defined as:
$N \cdot \begin{cases}e^{-t^{2} / 2} & \text { if } t>-\alpha_{C B}, \\ \left(\frac{n_{C B}}{\alpha_{C B}}\right)^{n_{C B}} \cdot e^{-\alpha_{C B}^{2} / 2} \cdot\left(\frac{n_{C B}}{\alpha_{C B}}-\alpha_{C B}-t\right)^{-n_{C B}} & \text { otherwise }\end{cases}$
where $t=\left(m_{\gamma \gamma}-\mu_{C B}\right) / \sigma_{C B}, N$ is a normalisation parameter, $\mu_{C B}$ is the peak of the narrow Gaussian distribution, $\sigma_{C B}$ represents the Gaussian resolution for the core component, and $n_{C B}$ and $\alpha_{C B}$ parametrise the non-Gaussian tail.

The core component of the mass resolution, $\sigma_{C B}$, ranges from 1.4 GeV in the "Unconverted central" category to 2.1 GeV in the "Converted transition" category. The non-Gaussian contributions to the mass resolution arise mostly from converted photons with at least one electron losing a significant fraction of its energy through bremsstrahlung in the inner detector material.

### 4.4. Sample composition

The main background components are the diphoton production, the photon-jet production with one fake photon from jets fragmenting into a high energy $\pi^{0}$, the dijet production with two fake photons, and Drell-Yan events where both electrons are misidentified as photons. A measurement of the diphoton production crosssection with 2010 ATLAS data can be found in Ref. [45], where the techniques used to estimate the purity of the sample are described in more detail. Although the final result does not rely on it, a quantitative understanding of the sample composition is an important cross-check of the diphoton selection procedure.

A method based on the use of control regions for two discriminating variables is applied to measure the contributions of fake photon background directly from the data. This method exploits relaxed isolation and photon identification cuts to estimate the fake components, by relying on the fact that the rejections from these two cuts are almost independent. It is a generalisation of the method used in Ref. [42]. The Drell-Yan background is estimated by measuring the probability for an electron to be reconstructed as a photon candidate with $Z$ events and applying this probability to the observed yield of Drell-Yan events at high mass.

The number of diphoton events in the $100-160 \mathrm{GeV}$ mass range is found to be $3650 \pm 100 \pm 290$, where the first uncertainty is sta-


Fig. 2. Diphoton, photon-jet, dijet and Drell-Yan contributions to the diphoton candidate invariant mass distribution, as obtained from a data-driven method. The various components are stacked on top of each other. The error bars correspond to the uncertainties on each component separately.
tistical and the second is systematic. The systematic uncertainty arises from the definition of the relaxed identification control region, the possible correlations between isolation and identification variables, and the fraction of real photons leaking into the background control regions. The extracted yields of photon-jet and dijet are $1110 \pm 60 \pm 270$ and $220 \pm 20 \pm 130$ events respectively. The Drell-Yan background, which is most prominent in the categories with at least one converted photon, is estimated to be $86 \pm 1 \pm 14$ events in the mass range of $100-160 \mathrm{GeV}$.

Fig. 2 shows the extracted components of the diphoton, photonjet, dijet and Drell-Yan processes. The purity of the sample (fraction of diphoton events) is about $72 \%$. The measurement of the purity has also been made separately in each category, and ranges from $69 \%$ to $83 \%$.

Other methods have been used to cross-check the purity estimate, in particular using template fits of the photon isolation distribution, where both signal and background templates are derived from data. The results are in agreement with the results quoted here.

## 5. Systematic uncertainties

Experimental systematic uncertainties affecting the extraction of the signal from the diphoton invariant mass distribution related to the modelling of the signal can be classified in two types: uncertainties affecting the predicted yield and uncertainties affecting the modelling of the mass resolution.

The uncertainties on the event yield are the following:

- The uncertainty from the photon reconstruction and identification efficiency amounts to $\pm 11 \%$ per event. It is estimated from data and MC differences in shower shape variables, the impact of additional material in front of the calorimeter and the impact of pileup on the photon shower shape variables.
- The uncertainty on the isolation cut efficiency is taken as the difference between data and MC found in $Z \rightarrow e e$ decays and amounts to $\pm 3 \%$ per event.
- The uncertainty on the photon trigger efficiency is $\pm 1 \%$. It comes from the uncertainty in the measurement of the trigger efficiency for diphoton candidates using control triggers and from possible differences between the trigger efficiency for photons from Higgs boson decays and all diphoton candidates.
- The uncertainty on the kinematic cut acceptance from the modelling of the Higgs boson transverse momentum distribu-
tion is investigated with HQT [46] and RESBOS [47,48], which account for all-orders soft-gluon resummation up to NNLL accuracy. The resulting uncertainty is found to be at the level of $\pm 1 \%$.
- The luminosity uncertainty is $3.7 \%$ [15].

The total uncertainty on the expected signal event yield is $\pm 12 \%$.
The uncertainties on the invariant mass resolution are the following:

- The uncertainty on the cluster energy resolution comes from the uncertainty on the sampling term, estimated to be $10 \%$, and from the uncertainty on the constant term, which is estimated using $Z \rightarrow$ ee decays. Both uncertainties are taken into account with their proper correlation from the Z control sample constraint. The uncertainty on the cluster energy resolution amounts to a $\pm 12 \%$ relative uncertainty on the diphoton invariant mass resolution.
- The uncertainty on the photon energy calibration arising from the extrapolation of the electron energy scale calibration is estimated from MC studies. The difference between the photon and the electron response in the calorimeter comes from the material in front of the active part of the calorimeter. The uncertainty is estimated using simulations with a different amount of material in front of the calorimeter and is found to be $\pm 6 \%$ on the mass resolution.
- The contribution of pileup fluctuations to the cluster energy measurement is checked using random clusters in randomly triggered bunch crossings, with a frequency corresponding to expectations from the instantaneous luminosity. The relative uncertainty on the mass resolution is found to be less than $3 \%$.
- The uncertainty on the resolution of the photon angle measurement is studied with $Z \rightarrow$ ee decays. The calorimeterbased direction measurement is compared with the much more precise track-based direction measurement. In the barrel calorimeter, the resolution measured in data agrees well with the one predicted by the simulation. In the end-cap region, the resolution measured in data is $\approx 20 \%$ worse than in the simulation. The impact of this difference is a $1 \%$ relative uncertainty on the diphoton mass resolution.

The total relative uncertainty on the diphoton invariant mass resolution is thus $\pm 14 \%$. This systematic uncertainty is applied to both the Crystal Ball and the wide Gaussian resolution parameters.

These systematic uncertainties are taken as fully correlated between the different categories. The impact of uncorrelated systematic uncertainties in the different categories and migration between categories has been investigated and found to be negligible.

The background is modelled by an exponentially falling invariant mass distribution. Systematic uncertainties arise from possible deviations of the background distribution from this assumed shape. This has been estimated by checking how accurately the chosen model fits different predicted diphoton mass distributions [49, 50] and comparing different functional forms for the background model. The resulting uncertainty is between $\pm 5$ events at 110 GeV and $\pm 3$ events at 150 GeV for a Higgs boson mass signal region about 4 GeV wide.

## 6. Results

The data are compared to background and signal-plus-background hypotheses using a profile likelihood test statistic as described in Refs. [7,51]. The exponentially falling invariant mass distribution used for the background model is determined by two

## Table 2

Fractions of background $\left(f_{b}\right)$, predicted signal $\left(f_{s}\right)$ and core Gaussian mass resolution $(\sigma)$ in each category for a Higgs boson mass hypothesis of 120 GeV . The fractions are normalised to the total yield summed over categories.

| Category | $f_{b}$ | $f_{s}$ | $\sigma(\mathrm{GeV})$ |
| :--- | ---: | :--- | :--- |
| Unconverted central | $7 \%$ | $15 \%$ | 1.4 |
| Unconverted rest | $29 \%$ | $27 \%$ | 1.6 |
| Converted central | $8 \%$ | $11 \%$ | 1.5 |
| Converted transition | $16 \%$ | $13 \%$ | 2.1 |
| Converted rest | $40 \%$ | $34 \%$ | 1.8 |



Fig. 3. Distribution of the reconstructed diphoton mass. All five diphoton categories have been combined. The exponential fit to the full sample of the background-only hypothesis, as well as the expected signal for a Higgs boson mass of 120 GeV with five times the Standard Model predicted yield, are also shown for illustration.
nuisance parameters per category (the normalisation and the exponential negative slope), which are left free in the unbinned fit. The signal is modelled with the mass resolution functions described above, one per category, fixing the fraction of events in each category to the MC predictions. Table 2 summarises the measured fractions of background events in each category, the predicted fractions of signal events and the predicted core Gaussian signal mass resolutions for a Higgs boson mass hypothesis of 120 GeV .

The fitted parameters for the signal are thus the overall signal strength relative to the Standard Model prediction and the nuisance parameters on the predicted event yield and mass resolution which have Gaussian constraints in the fit. The uncertainty on the predicted event yield includes both the experimental systematic uncertainties described in Section 5 and the uncertainty on the predicted cross-section described in Section 3. The systematic uncertainty on the background shape is included as another nuisance parameter with a Gaussian constraint in the fit. From this fit, the best estimate of the signal yield is extracted, as well as the likelihood ratio (profile likelihood) between any assumed signal yield (leaving the nuisance parameters free to maximise the likelihood) and the best estimate. The fit is performed in 1 GeV steps for the Higgs boson mass hypothesis, which is significantly smaller than the invariant mass resolution. The signal parameters for these fine mass steps are interpolated from the fully simulated samples.

Fig. 3 shows the reconstructed diphoton mass spectrum. No excess is visible. This is quantified by the $p$-value of the backgroundonly hypothesis, which gives the fraction of background-only experiments that would have a profile likelihood ratio of the zero signal hypothesis relative to the best-fitted signal strength at least as low as the one found in the data. Negative signals are not allowed in the fit, so $p$-values above 0.5 are truncated. This $p$-value is shown in Fig. 4(a) as a function of the hypothesised Higgs boson mass. The minimal $p$-value, corresponding to the largest back-


Fig. 4. (a) $p$-value ( $p_{0}$ ) of the background-only hypothesis as a function of the investigated Higgs boson mass; (b) $95 \%$ confidence level upper limits on a Standard Model Higgs boson production cross-section, relative to the Standard Model crosssection, as a function of Higgs boson mass hypothesis. The solid line shows the observed limit. The dashed line shows the median expected limit for background-only pseudo-experiments, with the bands indicating the expected fluctuations around this limit at the $1 \sigma$ and $2 \sigma$ levels.
ground upward fluctuation, is $\approx 5 \%$ and is found for a hypothesised mass of $\approx 128 \mathrm{GeV}$. The probability for such an excess to appear anywhere in the investigated mass range is around $40 \%$.

Exclusion limits on the inclusive production cross-section of a Standard Model Higgs boson relative to the Standard Model crosssection are derived. For this purpose, a modified frequentist approach $C L_{s}$ [52], corresponding to the ratio of $p$-values for the signal-plus-background and the background-only hypothesis for a given assumed signal strength is used. A given signal strength is excluded at $95 \%$ confidence level if its $C L_{s}$ is smaller than 0.05 . The confidence levels are computed using a large number of signal-plus-background pseudo-experiments, with different signal yields, and background-only pseudo-experiments. The results, including systematic uncertainties, are shown in Fig. 4(b). The impact of the experimental systematic uncertainties is about $5 \%$ on the expected limit for the mass hypothesis of 120 GeV .

The expected median limit in the case of no signal varies from 3.3 to 5.8 as a function of the Higgs boson mass. The variations of the observed limit, between 2.0 and 5.8 , are consistent with expected statistical fluctuations around the median limit.

## 7. Conclusions

A search for the Standard Model Higgs boson in the $H \rightarrow \gamma \gamma$ decay mode has been performed using an integrated luminosity of $1.08 \mathrm{fb}^{-1}$ recorded by the ATLAS experiment in 2011. A high purity diphoton sample is selected. No excess is found in the diphoton invariant mass distribution in the mass range of $110-150 \mathrm{GeV}$. The observed limit on the cross-section of a Standard Model-like Higgs
boson decaying into a pair of photons ranges between 2.0 and 5.8 times the Standard Model cross-section. These variations are compatible with statistical fluctuations around the expected limit for this data set. These limits are the most stringent to date in this channel.

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Grybel ${ }^{141}$, V.J. Guarino ${ }^{5}$, D. Guest ${ }^{175}$, C. Guicheney ${ }^{33}$, A. Guida ${ }^{72 \mathrm{a}, 72 \mathrm{~b}}$, T. Guillemin ${ }^{4}$, S. Guindon ${ }^{54}$, H. Guler ${ }^{85, n}$, J. Gunther ${ }^{125}$, B. Guo ${ }^{158}$, J. Guo ${ }^{34}$, A. Gupta ${ }^{30}$, Y. Gusakov ${ }^{65}$, V.N. Gushchin ${ }^{128}$, A. Gutierrez ${ }^{93}$, P. Gutierrez ${ }^{111}$, N. Guttman ${ }^{153}$, O. Gutzwiller ${ }^{172}$, C. Guyot ${ }^{136}$, C. Gwenlan ${ }^{118}$, C.B. Gwilliam ${ }^{73}$, A. Haas ${ }^{143}$, S. Haas ${ }^{29}$, C. Haber ${ }^{14}$, R. Hackenburg ${ }^{24}$, H.K. Hadavand ${ }^{39}$, D.R. Hadley ${ }^{17}$, P. Haefner ${ }^{99}$, F. Hahn ${ }^{29}$, S. Haider ${ }^{29}$, Z. Hajduk ${ }^{38}$, H. Hakobyan ${ }^{176}$, J. Haller ${ }^{54}$, K. Hamacher ${ }^{174}$, P. Hamal ${ }^{113}$, A. Hamilton ${ }^{49}$, S. Hamilton ${ }^{161}$, H. Han ${ }^{32 a}$, L. Han ${ }^{32 b}$, K. Hanagaki ${ }^{116}$, M. Hance ${ }^{120}$, C. Handel ${ }^{81}$, P. 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# Search for massive long-lived highly ionising particles with the ATLAS detector at the LHC ${ }^{\text {an }}$ 

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#### Abstract

A search is made for massive highly ionising particles with lifetimes in excess of 100 ns , with the ATLAS experiment at the Large Hadron Collider, using $3.1 \mathrm{pb}^{-1}$ of $p p$ collision data taken at $\sqrt{s}=7 \mathrm{TeV}$. The signature of energy loss in the ATLAS inner detector and electromagnetic calorimeter is used. No such particles are found and limits on the production cross section for electric charges $6 e \leqslant|q| \leqslant 17 e$ and masses $200 \mathrm{GeV} \leqslant m \leqslant 1000 \mathrm{GeV}$ are set in the range $1-12 \mathrm{pb}$ for different hypotheses on the production mechanism.


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## 1. Introduction

The observation of a massive long-lived highly ionising particle (HIP) possessing a large electric charge $|q| \gg e$, where $e$ is the elementary charge, would represent striking evidence for physics beyond the Standard Model. Examples of putative particles which can give rise to HIP signatures include $Q$-balls [1], stable micro black-hole remnants [2], magnetic monopoles [3] and dyons [4]. Searches for HIPs are made in cosmic rays [5] and at colliders [3]; recent collider searches were performed at LEP [6-8] and the Tevatron [9-12]. Cross sections and event topologies associated with HIP production cannot be reliably predicted due to the fact that the coupling between a HIP and the photon is so strong that perturbative calculations are not possible. Therefore, search results at colliders are usually quoted as cross section limits in a range of charge and mass for given kinematics [3]. Also, for the same reason, limits obtained at different collision energies or for different types of collisions cannot be directly compared; rather, they are complementary.

HIP searches are part of a program of searches at the CERN Large Hadron Collider (LHC) which explore the multi-TeV energy regime. Further motivation is provided by the gauge hierarchy problem, to which proposed solutions typically postulate the existence of hitherto unobserved particles with TeV-scale masses. HIPs at the LHC can be sought at the dedicated MoEDAL plastic-track experiment [13] or, as in this work, via their active detection at a multipurpose detector.

[^6]Due to their assumed large mass (hundreds of GeV), HIPs are characterised by their non-relativistic speed. The expected large amounts of energy loss per unit length ( $\mathrm{d} E / \mathrm{d} x$ ) through ionisation (no bremsstrahlung) are mainly due to the high particle charge, but also due to the low speed. The ATLAS detector is well suited to detect HIPs. A HIP with sufficient kinetic energy would leave a track in the inner detector tracking system of ATLAS and lose its energy on its way to and through the electromagnetic calorimeter, giving rise to an electron-like signature. The presence of a HIP can be inferred from measurements of the proportion of high-ionisation hits in the inner detector. In addition, assuming isolation, the lateral extent of the energy deposition in the calorimeter is a sensitive discriminant between HIPs and Standard Model particles.

The ranges of HIP charge, mass and lifetime for which unambiguous conclusions can be drawn are determined by the chosen trigger and event selections. The choice of an electromagnetic trigger limits the phase space to HIPs which stop in the electromagnetic calorimeter of ATLAS. The search is optimised for data collected at relatively low instantaneous luminosities (up to $10^{31} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ ), for which a low ( 10 GeV ) trigger transverse energy threshold is available. In the barrel region of the calorimeter, this gives access to energy depositions corresponding to HIPs with electric charges down to $6 e$. Standard electron reconstruction algorithms are used, which implies that tracks which bend like electrically charged particles are sought. Particles with magnetic charge, or electric charge above $17 e$, are not addressed here due to the bending along the beam axis in the case of a monopole, and due to effects from delta electrons and electron recombination in the active detector at the corresponding values of energy loss ( $\mathrm{d} E / \mathrm{d} x>2 \cdot 10^{3} \mathrm{MeV} / \mathrm{cm}$ ). For such types of HIPs, more detailed studies are needed to assess and minimise the impact of these
effects on the selection efficiency. The 1000 GeV upper bound in mass sensitivity is determined by trigger timing constraints, as a significantly heavier HIP (with charge 17e or lower) would be delayed by more than 12 ns with respect to $\beta=1$ when it stops in the electromagnetic calorimeter (this corresponds to $\beta<0.3$ ), and would thus risk being triggered in the next proton bunch crossing. The search is sensitive to HIP lifetimes larger than 100 ns since a particle which decays much earlier in the calorimeter (even after stopping) would spoil the signature of a narrow energy deposition.

## 2. The ATLAS detector

The ATLAS detector [14] is a multipurpose particle physics apparatus with a forward-backward symmetric cylindrical geometry and near $4 \pi$ coverage in solid angle. ${ }^{1}$ A thin superconducting solenoid magnet surrounding the inner part of the ATLAS detector produces a field of approximately 2 T along the beam axis.

Inner detector (ID) tracking is performed by silicon-based detectors and an outer tracker using straw tubes with particle identification capabilities based on transition radiation (Transition Radiation Tracker, TRT). The TRT is divided into barrel (covering the pseudorapidity range $|\eta|<1.0$ ) and endcap ( $0.8<|\eta|<2.0$ ) components. A track gives a typical number of straw hits of 36 . At the front-end electronics of the TRT, discriminators are used to compare the signal against low and high thresholds. While the TRT has two hit threshold levels, there is no upper limit to the amount of ionisation in a straw which will lead to a signal [15], guaranteeing that highly ionising particles would not escape detection in the TRT. Rather, they would produce a large number of high-threshold (HT) hits along their trajectories. The amount of ionisation in a straw tube needed for a TRT HT hit is roughly equivalent to three times that expected from a minimum ionising particle.

Liquid-argon sampling electromagnetic (EM) calorimeters, which comprise accordion-shaped electrodes and lead absorbers, surround the ID. The EM calorimeter barrel ( $|\eta|<1.475$ ) is used in this search. It is segmented transversely and divided in three layers in depth, denoted first, second, and third layer, respectively. In front of the accordion calorimeter a thin presampler layer is used to correct for fluctuations of energy loss. The typical cell granularity $(\Delta \eta \times \Delta \phi)$ of the EM barrel is $0.003 \times 0.1$ in the first layer and $0.025 \times 0.025$ in the second layer. The signal expected for a HIP in the considered charge range lies in a region in time and energy where the electronic response in EM calorimeter cells is well understood and does not saturate. The robustness of the EM calorimeter energy reconstruction has been studied in detail and pulse shape predictions are consistent with the measured signals [16].

The stopping power of a HIP in the ATLAS detector depends on its charge, mass and energy, as well as the material budget along its path. Details of the latter are given in Ref. [17] in terms of number of radiation lengths $X_{0}$, as a function of depth and pseudorapidity. The integrated radiation length between the interaction point and the exit of the TRT is $0.5 X_{0}$ at $\eta=0$ and $1.5 X_{0}$ at $|\eta|=1.3$. The additional amount of material before the first layer of the EM calorimeter is $2.0 X_{0}$ at $\eta=0$ and $3.5 X_{0}$ at $|\eta|=1.3$. The thicknesses of the first, second and third EM layers are $4.5 X_{0}$, $16.5 X_{0}$ and $1.5 X_{0}$ at $\eta=0$ and $3 X_{0}, 20 X_{0}$ and $5 X_{0}$ at $|\eta|=1.3$, respectively.

[^7]

Fig. 1. Distributions of pseudorapidity $\eta$ (top) and kinetic energy $E_{\text {kin }}$ (bottom) at origin for heavy fermions produced with the Drell-Yan process. The latter is given with a requirement of $|\eta|<1.35$. The distributions for the three different masses are normalised to the same number of entries.

## 3. Simulated event samples

Signal events are generated with the Pythia Monte Carlo (MC) event generator [18] according to the fermion pair production process: $p+p \rightarrow f+\bar{f}+X$. Ref. [19] is used for the parton distributions of the proton. Direct pair production implies that the HIPs are not part of a jet and thus isolated. A Drell-Yan-like production mechanism, modified to take into account the mass of the HIP [20], is used to model the kinematic properties of the HIPs. Generated $\eta$ distributions, as well as kinetic energy ( $E_{k i n}$ ) spectra in the central region ( $|\eta|<1.35$ ), are shown in Fig. 1 for the three mass points considered in this search.

An ATLAS detector simulation [21] based on Geant-4 [22] is used, where the particle interactions include secondary ionisation by delta electrons in addition to the standard ionisation process based on the Bethe-Bloch formula. A correction for electron-ion recombination effects in the EM calorimeter (Birks' correction) is applied, with typical visible energy fractions between 0.2 and 0.5 for the signal particles considered. Effects of delays are simulated, except for the ability to trigger slow-moving particles within the proton bunch crossing time, which is considered separately as a systematic uncertainty (see Section 6). Samples of approximately 20000 events are produced for HIPs with masses of 200, 500 and 1000 GeV . For each mass point, HIPs with charges $6 e, 10 e$ and $17 e$ are simulated.

A data-driven method is used in this work to estimate backgrounds surviving the final selections (see Section 4.2). However, in order to demonstrate that the distributions of the relevant observables are understood, a sample of simulated background events is used. The background sample, generated with Pythia [18] and labeled "Standard Model", consists mostly of QCD events in which
the hard subprocess is a strong 2 -to-2 process with a matrix element transverse momentum cut-off of 15 GeV , but also includes contributions from heavy quark and vector boson production. A true transverse energy larger than 17 GeV in a typical first level trigger tower is also required. This sample contains $4 \cdot 10^{7}$ events and corresponds roughly to an integrated luminosity of $0.8 \mathrm{pb}^{-1}$.

## 4. Trigger and event selection

The collected data sample corresponds to an integrated luminosity of $3.1 \pm 0.3 \mathrm{pb}^{-1}$, using a first level trigger based on energy deposits in the calorimeters. At the first level of the trigger, socalled trigger towers with dimension $\Delta \eta \times \Delta \phi=0.1 \times 0.1$ are defined. In each trigger tower the cells of the electromagnetic or hadronic calorimeter are summed. EM clusters with fixed size $\Delta \eta \times \Delta \phi=0.2 \times 0.2$ are sought and are retained if the total transverse energy ( $E_{T}$ ) in an adjacent pair of their four trigger towers is above 5 GeV . Further electron-like higher level trigger requirements are imposed on the candidate, including $E_{T}>10 \mathrm{GeV}$, a matching to a track in the ID and a veto on hadronic leakage [23]. The efficiency of this trigger for the data under consideration is measured to be $(94.0 \pm 1.5) \%$ for electrons with $E_{T}>15 \mathrm{GeV}$ and is well described by the simulation. The simulation predicts that a highly charged particle which stops in the EM barrel would be triggered with a similar efficiency or higher.

Offline electron candidates have cluster sizes of $\Delta \eta \times \Delta \phi=$ $0.075 \times 0.175$ in the EM barrel, with a matched track in a window of $\Delta \eta \times \Delta \phi=0.05 \times 0.1$ amongst reconstructed tracks with transverse momentum larger than 0.5 GeV . Identification requirements corresponding to "medium" electrons [24], implying track and shower shape quality cuts, are applied to the candidates. These cuts filter out backgrounds but have a negligible impact on the signal, for which the cluster width is much narrower than for typical electrons. The cluster energy is estimated correcting for the energy deposited outside the active calorimeter regions, assuming an EM shower.

Further offline selections on the cluster transverse energy ( $E_{T}>$ 15 GeV ) and pseudorapidity ( $|\eta|<1.35$ ) are imposed. The $E_{T}$ selection guarantees that the trigger efficiency is higher than $94 \%$ for the objects under study. The restriction of $|\eta|<1.35$ excludes the transition region between the EM calorimeter barrel and endcap, reducing the probability for backgrounds to fake a narrow energy deposition.

### 4.1. Selection cuts

A loose selection based on TRT and EM calorimeter information is also imposed on the candidates to ensure that the quality of the track and cluster associated to the electron-like object is good enough to ensure the robustness of the HIP selection variables, and to provide a data sample with which to estimate the background rate. Only candidates with more than 10 TRT hits are retained. In addition to the $E_{T}>15 \mathrm{GeV}$ cut for the EM cluster associated with the candidate, a significant fraction of the total cluster energy is required to be contained in six calorimeter cells among the first and second EM layers. This is done by requiring the summed energy in the three most energetic cells in each of the first and second layers to be greater than 2 and 4 GeV , respectively. Following these selections, 137503 candidates remain in the data.

Two sets of observables are used in the final selection. The ID-based observable is the fraction, $f_{H T}$, of TRT hits on the track which pass the high threshold. The calorimeter-based discriminants are the fractions of energies outside of the three most energetic cells associated to a selected EM cluster, in the first and second EM calorimeter layers: $w_{1}$ and $w_{2}$.


Fig. 2. Distribution of the fraction of TRT high-threshold hits for candidates satisfying the loose selection. Data (dots) are compared with area-normalised signal ( $|q|=10 e$ and $m=500 \mathrm{GeV}$, dashed line) and Standard Model background (shaded area) simulations. The dotted line shows the selection cut value.

The $f_{H T}$ distribution for loosely selected candidates is shown in Fig. 2. The data extend up to $f_{H T}=0.8$. The prediction of the signal simulation for a HIP of mass 500 GeV and charge $10 e$ is also shown. It peaks at $f_{H T} \sim 1$ and has a small tail extending into the Standard Model region.

The distributions of $w_{1}$ and $w_{2}$ also provide good discrimination between signal and background, as shown in Fig. 3. For a signal, energy is deposited only in the few cells along the particle trajectory (as opposed to backgrounds which induce showers in the EM calorimeter) and the distributions peak around zero for both variables. The shapes of the measured distributions are well described by the background simulation. A faint double-peak structure is visible in data and in background simulations for the $f_{H T}$, $w_{1}$ and $w_{2}$ distributions in Figs. 2 and 3, where the main peak (closest to the signal) corresponds to electrons and the secondary peak corresponds to hadrons which fake the electron identification signature.

Finally, the following HIP selection is made: $f_{H T}>0.65, w_{1}<$ 0.20 and $w_{2}<0.15$. For signal particles, these cuts reject only candidates in the tails of the distributions, and varying them has a minor impact on the efficiency; this feature is common to all considered charge and mass points. The cut values were chosen to yield a very small ( $\ll 1$ event) expected background (see Section 4.2) while retaining a high ( $\sim 96 \%$ ) efficiency for the signal. No candidates in data or in simulated Standard Model events pass this selection.

### 4.2. Data-driven background estimation

A data-driven method is used to quantify the expected background yield after the HIP selection. Potential backgrounds consist mainly of electrons. For Standard Model candidates, the ID and calorimeter observables are correlated in a way that further suppresses the backgrounds (see Fig. 4). The background estimation assumes that $f_{H T}$ is uncorrelated with $w_{1}$ and $w_{2}$ and is thus conservative.

The yield of particle candidates passing the loose selection $N_{\text {loose }}=137503$ can be divided into the following: $N_{0}, N_{1}, N_{f_{H T}}$, and $N_{w}$, which represent the number of candidates which satisfy both of the selections, neither of the selections, only the $f_{H T}$ selection, and only the $w_{1}$ and $w_{2}$ selections taken together, respectively. Even in the presence of a signal, $N_{1}, N_{f_{H T}}$ and $N_{w}$ would be dominantly composed of background events. The probability of a background candidate passing the TRT requirement is


Fig. 3. Distributions of $w_{1}$ and $w_{2}$ following the loose selection. Data (dots) are compared with area-normalised signal ( $|q|=10 e$ and $m=500 \mathrm{GeV}$, dashed lines) and Standard Model background (shaded area) simulations. Negative values are caused by pedestal fluctuations. Dotted lines show the selection cut values.
then $P_{f_{H T}}=\frac{N_{f_{H T}}}{\left(N_{1}+N_{f_{H T}}\right)}$ and the probability to pass the calorimeter requirements is $P_{w}=\frac{N_{w}}{\left(N_{1}+N_{w}\right)}$, leading to an expectation of the number of background candidates entering the signal region: $N_{b g}=N_{\text {loose }} P_{f_{H T}} P_{w}$. The data sample yields $N_{0}=0, N_{1}=137342$, $N_{f_{H T}}=18$ and $N_{w}=143$, leading to $P_{f_{H T}}=(1.3 \pm 0.3) \cdot 10^{-4}$ and $P_{w}=(1.0 \pm 0.1) \cdot 10^{-3}$. The expected number of background candidates surviving the selection, and thereby the expected number of background events, is thus $N_{b g}=0.019 \pm 0.005$. The quoted uncertainty is statistical.

## 5. Signal selection efficiency

### 5.1. Efficiencies in acceptance kinematic regions

The probability to retain a signal event can be factorised in two parts: acceptance (probability for a HIP in a region where the detector is sensitive) and efficiency (probability for this HIP to pass the selection cuts). The acceptance is defined here as the probability that at least one signal particle will be in the range $|\eta|<1.35$ and stop in the second or third layer of the EM calorimeter. If this condition is satisfied, the simulation predicts a high probability to trigger on, reconstruct and select the event. This corresponds to the dark region in Fig. 5, which shows the predicted selection efficiency mapped as a function of the initial HIP pseudorapidity and kinetic energy, in the case of $|q|=10 e$ and $m=500 \mathrm{GeV}$. Such acceptance kinematic regions can be parametrised with three values defining three corners of a parallelogram. These parameters are summarised in Table 1. For HIPs produced inside such regions, the


Fig. 4. Contours of $w_{2}$ versus $f_{H T}$ distributions following loose selection, showing the density of entries on a log scale. Data and signal Monte Carlo ( $|q|=10 e$ and $m=500 \mathrm{GeV}$ ) are shown, and no candidates in the data appear near the signal region. The correlation factor between $w_{2}$ and $f_{H T}$ in the data is positive (coefficient 0.15 ); the same trend is also true for the correlation between $w_{1}$ and $f_{H T}$ (coefficient 0.18 ).

Table 1
Kinetic energies (in GeV ) defining the acceptance kinematic ranges for HIPs with the masses and electric charges considered in this search. The three columns correspond to the lower left, lower right, and upper left corners of parallelograms in the ( $|\eta|, E_{k i n}$ ) plane.

| $\|q\|$ | $m[\mathrm{GeV}]$ | $E_{\text {kin }}^{\min }$ <br> $(\eta=0)$ | $E_{\text {kin }}^{\min }$ <br> $(\|\eta\|=1.35)$ | $E_{\text {kin }}^{\max }$ <br> $(\eta=0)$ |
| :---: | :---: | :---: | :---: | :---: |
| $6 e$ | 200 | 40 | 50 | 50 |
| $6 e$ | 500 | 50 | 70 | 70 |
| $6 e$ | 1000 | 60 | 130 | 80 |
| $10 e$ | 200 | 50 | 80 | 90 |
| $10 e$ | 500 | 80 | 110 | 130 |
| $10 e$ | 1000 | 110 | 150 | 180 |
| $17 e$ | 200 | 100 | 150 | 190 |
| $17 e$ | 500 | 150 | 190 | 260 |
| $17 e$ | 1000 | 190 | 240 | 350 |

Table 2
Expected fractions of HIP candidates passing the final selection, assuming they are isolated and produced inside the acceptance regions defined by the values in Table 1. Uncertainties due to MC statistics are quoted; other systematic uncertainties are discussed in Section 6.

| $m[\mathrm{GeV}]$ | $\|q\|=6 e$ | $\|q\|=10 e$ | $\|q\|=17 e$ |
| :---: | :--- | :--- | :--- |
| 200 | $0.822 \pm 0.026$ | $0.820 \pm 0.015$ | $0.484 \pm 0.012$ |
| 500 | $0.868 \pm 0.021$ | $0.856 \pm 0.014$ | $0.617 \pm 0.011$ |
| 1000 | $0.558 \pm 0.019$ | $0.858 \pm 0.012$ | $0.700 \pm 0.012$ |

candidate selection efficiency is flat within $10 \%$ and takes values between 0.5 and 0.9 depending on the charge and mass (see Table 2 ). For $|q|=17 e$, the main source of inefficiency is the requirement on the number of TRT HT hits, which contributes up to $20 \%$ signal loss. This is largely due to the presence of track segments from delta electrons, which have a non-negligible probability to be chosen by the standard electron track matching algorithm. For low charges, inefficiencies are dominated by the cluster $E_{T}$ cut, typically accounting for $\sim 6 \%$ loss. Other contributions, like trigger, electron reconstruction, and electron identification, can each cause $1-6 \%$ additional inefficiency.

### 5.2. Efficiencies for Drell-Yan kinematics

The estimated fractions of signal events where at least one candidate passes the final selection, assuming they are produced


Fig. 5. Probability to pass all selection criteria as a function of pseudorapidity and kinetic energy at origin, for a HIP with charge $10 e$ and mass 500 GeV . The dark region corresponds to the kinetic range where the particle stops in or near the second layer of the EM calorimeter barrel and is parametrised with three energy values (dashed parallelogram, see Table 1).

Table 3
Expected fractions of signal events passing the final selection, assuming Drell-Yan kinematics. Uncertainties due to MC statistics are quoted; other systematic uncertainties are discussed in Section 6.

| $m[\mathrm{GeV}]$ | $\|q\|=6 e$ | $\|q\|=10 e$ | $\|q\|=17 e$ |
| :---: | :--- | :--- | :--- |
| 200 | $0.102 \pm 0.002$ | $0.175 \pm 0.003$ | $0.112 \pm 0.002$ |
| 500 | $0.150 \pm 0.003$ | $0.236 \pm 0.003$ | $0.193 \pm 0.003$ |
| 1000 | $0.133 \pm 0.002$ | $0.299 \pm 0.004$ | $0.237 \pm 0.004$ |

with Drell-Yan kinematics, are shown in Table 3 for the values of charge and mass considered in this search. The dominant source of loss ( $70-85 \%$ loss) is from the kinematic acceptance, i.e., the production of HIPs with $|\eta|>1.35$, as well as their stopping before they reach the second layer of the EM calorimeter, or after they reach the first layer of the hadronic calorimeter. The relative contributions from these various types of acceptance loss depend on mass and charge, as well as the kinematics of the assumed production model. The Drell-Yan production model implies that the fraction of HIPs produced in the acceptance region of pseudorapidity $|\eta|<1.35$ is larger with increasing mass (see Fig. 1). Also, with the assumed energy spectra (bottom plot in Fig. 1), the acceptance is highest for intermediate charges ( $|q|=10 e$ ), since HIPs with low charges tend to punch through the EM calorimeter and HIPs with high charges tend to stop before reaching it.

## 6. Systematic uncertainties

The major sources of systematic uncertainties affecting the efficiency estimation are summarised below. These mainly concern possible imperfections in the description of HIPs in the detector by the simulation.

- The recombination of electrons and ions in the sampling region of the EM calorimeter affects the measured current and thus the total visible energy. Recombination effects become larger with increasing $\mathrm{d} E / \mathrm{d} x$. In the ATLAS simulation, this is parametrised by Birks' law [25]. To estimate the uncertainty associated with the approximate modeling of recombination effects, predictions from the ATLAS implementation of Birks' correction [26] are compared to existing data of heavy ions punching through a layer of liquid argon [27-29]. In the range $2 \cdot 10^{2} \mathrm{MeV} / \mathrm{cm}<\mathrm{d} E / \mathrm{d} x<2 \cdot 10^{3} \mathrm{MeV} / \mathrm{cm}$, which corresponds to typical HIP energy losses in the EM calorimeter for the

Table 4
Relative systematic uncertainties in efficiency, combining in quadrature all the effects described in the text.

| $m[\mathrm{GeV}]$ | $\|q\|=6 e$ | $\|q\|=10 e$ | $\|q\|=17 e$ |
| :---: | :--- | :--- | :--- |
| 200 | $25 \%$ | $11 \%$ | $9 \%$ |
| 500 | $17 \%$ | $10 \%$ | $9 \%$ |
| 1000 | $28 \%$ | $10 \%$ | $9 \%$ |

charges and masses under consideration, the uncertainty in the simulated visible energy fraction is $\pm 15 \%$. This introduces between $4 \%$ and $23 \%$ uncertainty in the signal selection efficiency. The impact is largest for charge $6 e$, for which a lower visible energy would be more likely to push the candidate below the 15 GeV cluster $E_{T}$ threshold.

- The fraction of HIPs which stop in the detector prior to reaching the EM calorimeter is affected by the assumed amount of material in the Geant-4 simulation. Varying the material density within the assumed uncertainty range ( $\pm \sim 10 \%$ [30]), independently in the ID and EM calorimeter volumes, leads to a $6 \%$ uncertainty in signal acceptance.
- The modeling of inactive or inefficient EM calorimeter regions in the simulation results in a $2 \%$ uncertainty in the signal efficiency.
- Cross-talk effects between EM calorimeter cells affect the $w_{1}$ and $w_{2}$ variables and this may not be accurately described by the simulation for large energy depositions per cell. The resulting uncertainty in signal efficiency is $2 \%$.
- Secondary ionisation by delta electrons affects the track reconstruction and the calorimeter energy output. The amount of delta electrons in ATLAS detectors as described in Geant-4 depends on the cutoff parameter (the radius beyond which delta electrons are considered separate from the mother particle). Varying this parameter results in a $3 \%$ uncertainty in the signal efficiency.
- For clusters delayed by more than 10 ns with respect to the expected arrival time of a highly relativistic particle, which corresponds to $\beta<0.37$, there is a significant chance that the event is triggered in the next bunch crossing by the first level EM trigger. In most of the mass and charge range considered in this search, more than $99 \%$ of the particles which are energetic enough to reach the EM calorimeter and pass the event selection are in the high-efficiency range $\beta>0.4$. The only exception is $|q|=6 e$ and $m=1000 \mathrm{GeV}$, for which the $\beta$ distribution after selection peaks between 0.32 and 0.47 . The trigger efficiency loss is corrected for, resulting in an additional $25 \%$ uncertainty for this particular case.
- Uncertainties in the choice of parametrisation for the parton density functions (pdfs) of the proton have an impact on the event kinematics. To test this effect, events were generated (see Section 3) with 7 different pdfs from various sources [19, 31-34]. Assuming that acceptance variations due to the choice of pdf are Gaussian, the resulting relative uncertainty in the acceptance is $3 \%$.
- The relative uncertainty in efficiency due to MC statistics is of the order of $2 \%$.

Other effects, like event pile-up and electron pick-up by positively charged particles, have been investigated and found to be negligible. Efficiency systematics are dominated by Birks' correction. The relative uncertainties in the signal selection efficiencies (Tables 2 and 3), obtained by adding all effects in quadrature, are shown in Table 4.

The systematic uncertainty in the absolute integrated luminosity is $11 \%$ [35].

Table 5
Inclusive HIP cross section upper limits (in pb) at 95\% confidence level for isolated long-lived massive particles with high electric charges produced in regions of pseudorapidity and kinetic energy as defined in Table 1. Efficiencies in Table 2 and uncertainties in Table 4 were used in the cross section limit calculation.

| $m[\mathrm{GeV}]$ | $\|q\|=6 e$ | $\|q\|=10 e$ | $\|q\|=17 e$ |
| :---: | :--- | :--- | :--- |
| 200 | 1.4 | 1.2 | 2.1 |
| 500 | 1.2 | 1.2 | 1.6 |
| 1000 | 2.2 | 1.2 | 1.5 |

Table 6
Pair production cross section upper limits (in pb) at $95 \%$ confidence level for longlived massive particles with high electric charges, assuming a Drell-Yan mechanism. Efficiencies in Table 3 and uncertainties in Table 4 were used in the cross section limit calculation.

| $m[\mathrm{GeV}]$ | $\|q\|=6 e$ | $\|q\|=10 e$ | $\|q\|=17 e$ |
| :---: | :---: | :--- | :--- |
| 200 | 11.5 | 5.9 | 9.1 |
| 500 | 7.2 | 4.3 | 5.3 |
| 1000 | 9.3 | 3.4 | 4.3 |

## 7. Upper limit on the cross section

A very low ( $\ll 1$ event) background yield is expected and no events are observed to pass the selection. Knowing the integrated luminosity ( $3.1 \mathrm{pb}^{-1}$ ) and the selection efficiency for various model assumptions (Tables 2 and 3 ), cross section limits are obtained. This is done using a Bayesian statistical approach with a uniform prior for the signal and the standard assumption that the uncertainties in integrated luminosity (11\%) and efficiency (Table 4) are Gaussian and independent. The limits are presented in Table 5 (for a particle produced in the acceptance kinematic region defined by Table 1) and in Table 6 (assuming Drell-Yan kinematics).

These limits can be approximately interpolated to intermediate values of mass and charge. Also, the limits quoted in Table 5 can be used to extract cross section limits for any given model of kinematics by correcting for the acceptance (fraction of events with at least one generated HIP in the ranges defined by Table 1): such a procedure yields conservative limits thanks to the fact that candidates beyond the sharp edges of the acceptance regions defined in Table 1 can also be accepted.

## 8. Summary

A search has been made for HIPs with lifetimes in excess of 100 ns produced in the ATLAS detector at the LHC using $3.1 \mathrm{pb}^{-1}$ of $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$. The signature of high ionisation in an inner detector track matched to a narrow calorimeter cluster has been used. Upper cross section limits between 1.2 pb and 11.5 pb have been extracted for HIPs with electric charges between $6 e$ and $17 e$ and masses between 200 GeV and 1000 GeV , under two kinematics assumptions: a generic isolated HIP in a fiducial range of pseudorapidity and kinetic energy, or a Drell-Yan fermion pair production mechanism. HIP mass ranges above 800 GeV [11] are probed for the first time at a particle collider. These limits are the first constraints obtained on long-lived highly charged particle production at LHC collision energies.

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V. Malyshev ${ }^{107}$, S. Malyukov ${ }^{65}$, R. Mameghani ${ }^{98}$, J. Mamuzic ${ }^{12 b}$, A. Manabe ${ }^{66}$, L. Mandelli ${ }^{89 a}$, I. Mandić ${ }^{74}$, R. Mandrysch ${ }^{15}$, J. Maneira ${ }^{124 a}$, P.S. Mangeard ${ }^{88}$, I.D. Manjavidze ${ }^{65}$, A. Mann ${ }^{54}$, P.M. Manning ${ }^{137}$, A. Manousakis-Katsikakis ${ }^{8}$, B. Mansoulie ${ }^{136}$, A. Manz ${ }^{99}$, A. Mapelli ${ }^{29}$, L. Mapelli ${ }^{29}$, L. March ${ }^{80}$, J.F. Marchand ${ }^{29}$, F. Marchese ${ }^{133 a, 133 b}$, M. Marchesotti ${ }^{29}$, G. Marchiori ${ }^{78}$, M. Marcisovsky ${ }^{125}$, A. Marin ${ }^{21, *}$, C.P. Marino ${ }^{61}$, F. Marroquim ${ }^{23 a}$, R. Marshall ${ }^{82}$, Z. Marshall ${ }^{34, m}$, F.K. Martens ${ }^{158}$, S. Marti-Garcia ${ }^{167}$, A.J. Martin ${ }^{175}$, B. Martin ${ }^{29}$, B. Martin ${ }^{88}$, F.F. Martin ${ }^{120}$, J.P. Martin ${ }^{93}$, Ph. Martin ${ }^{55}$, T.A. Martin ${ }^{17}$, B. Martin dit Latour ${ }^{49}$, M. 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# Search for high mass dilepton resonances in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS experiment ${ }^{*}$ 

ATLAS Collaboration*

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#### Abstract

This Letter presents a search for high mass $e^{+} e^{-}$or $\mu^{+} \mu^{-}$resonances in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ at the LHC. The data were recorded by the ATLAS experiment during 2010 and correspond to a total integrated luminosity of $\sim 40 \mathrm{pb}^{-1}$. No statistically significant excess above the Standard Model expectation is observed in the search region of dilepton invariant mass above 110 GeV . Upper limits at the $95 \%$ confidence level are set on the cross section times branching ratio of $Z^{\prime}$ resonances decaying to dielectrons and dimuons as a function of the resonance mass. A lower mass limit of 1.048 TeV on the Sequential Standard Model $Z^{\prime}$ boson is derived, as well as mass limits on $Z^{*}$ and $E_{6}$-motivated $Z^{\prime}$ models.


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A search for high mass resonances decaying into $e^{+} e^{-}$or $\mu^{+} \mu^{-}$pairs is presented based on an analysis of $7 \mathrm{TeV} p p$ collision data recorded with the ATLAS detector [1]. Among the possibilities for such resonances, this Letter focuses on new heavy neutral gauge bosons ( $Z^{\prime}, Z^{*}$ ) [2-4]; other hypothetical states like a Randall-Sundrum spin-2 graviton [5] or a spin-1 techni-meson [6] are not discussed here, though this analysis is also sensitive to them.

The benchmark model for $Z^{\prime}$ bosons is the Sequential Standard Model (SSM) [2], in which the $Z^{\prime}\left(Z_{\text {SSM }}^{\prime}\right)$ has the same couplings to fermions as the $Z$ boson. A more theoretically motivated model is the Grand Unification model in which the $E_{6}$ gauge group is broken into $S U(5)$ and two additional $U(1)$ groups [7]. The lightest linear combination of the corresponding two new neutral gauge bosons, $Z_{\psi}^{\prime}$ and $Z_{\chi}^{\prime}$, is considered the $Z^{\prime}$ candidate: $Z^{\prime}\left(\theta_{E_{6}}\right)=Z_{\psi}^{\prime} \cos \theta_{E_{6}}+Z_{\chi}^{\prime} \sin \theta_{E_{6}}$, where $0 \leqslant \theta_{E_{6}}<\pi$ is the mixing angle between the two gauge bosons. The pattern of spontaneous symmetry breaking and the value of $\theta_{E_{6}}$ determines the $Z^{\prime}$ couplings to fermions; six different models [2,7] lead to the specific $Z^{\prime}$ states named $Z_{\psi}^{\prime}, Z_{N}^{\prime}, Z_{\eta}^{\prime}, Z_{I}^{\prime}, Z_{S}^{\prime}$ and $Z_{\chi}^{\prime}$ respectively. Because of different couplings to $u$ and $d$ quarks, the ranking of the production cross sections of these six states is different in $p \bar{p}$ and $p p$ collisions. In this search, the resonances are assumed to have a narrow intrinsic width, comparable to the contribution from the

[^8]detector mass resolution. The expected intrinsic width of the $Z_{\mathrm{SSM}}^{\prime}$ as a fraction of the mass is $3.1 \%$, while for any $E_{6}$ model the intrinsic width is predicted to be between $0.5 \%$ and $1.3 \%$ [8].

Production of a $Z^{*}$ boson $[4,9]$ could also be detected in a dilepton resonance search. The anomalous (magnetic moment type) coupling of the $Z^{*}$ boson leads to kinematic distributions different from those of the $Z^{\prime}$ boson. To fix the coupling strength, a model with quark-lepton universality, and with the total $Z^{*}$ decay width equal to that of the $Z_{\text {SSM }}^{\prime}$ with the same mass, is adopted [10,11].

Previous indirect and direct searches have set constraints on the mass of $Z^{\prime}$ resonances [12-16]. The $Z_{S S M}^{\prime}$ is excluded by direct searches at the Tevatron with a mass lower than $1.071 \mathrm{TeV}[17,18]$. The large center of mass energy of the LHC provides an opportunity to search for $Z^{\prime}$ resonances with comparable sensitivity using the $2010 p p$ collision data. CMS has very recently excluded a $Z_{\text {SSM }}^{\prime}$ with a mass lower than 1.140 TeV [19].

The three main detector systems of ATLAS [1] used in this analysis are the inner tracking detector, the calorimeter, and the muon spectrometer. Charged particle tracks and vertices are reconstructed with the inner detector (ID) which consists of silicon pixel, silicon strip, and transition radiation detectors covering the pseudorapidity range $|\eta|<2.5$. ${ }^{1}$ It is immersed in a homogeneous

[^9]2 T magnetic field provided by a superconducting solenoid. The latter is surrounded by a finely-segmented, hermetic calorimeter that covers $|\eta|<4.9$ and provides three-dimensional reconstruction of particle showers using lead-liquid argon sampling for the electromagnetic compartment followed by a hadronic compartment which is based on iron-scintillating tiles sampling in the central region and on liquid argon sampling with copper or tungsten absorbers for $|\eta|>1.7$. Outside the calorimeter, there is a muon spectrometer with air-core toroids providing a magnetic field. Three sets of drift tubes or cathode strip chambers provide precision $(\eta)$ coordinates for momentum measurement in the region $|\eta|<2.5$. Finally, resistive-plate and thin-gap chambers provide muon triggering capability.

The data sample used in this analysis was collected during 2010. Application of detector and data quality requirements leads to an available integrated luminosity of $39 \mathrm{pb}^{-1}$ and $42 \mathrm{pb}^{-1}$ for the electron and muon analyses respectively.

Triggers requiring the presence of at least one electron or muon above a transverse momentum ( $p_{\mathrm{T}}$ ) threshold were used to identify the events recorded for full reconstruction. The thresholds varied from 14 to 20 GeV for electrons and 10 to 13 GeV for muons depending on the luminosity. The overall trigger efficiency at the $Z$ peak is $100 \%$ with negligible uncertainty for dielectron events and $(98.2 \pm 0.3) \%$ for dimuon events, for the selection criteria presented below. The trigger-level bunch-crossing identification of very high transverse energy electron triggers relies on a special algorithm implemented in the first-level calorimeter trigger hardware; its performance was checked with calibration data and the resulting systematic uncertainty on the trigger efficiency is ${ }_{-2}^{+0} \%$. Collision candidates are selected by requiring a primary vertex with at least three associated charged particle tracks, consistent with the beam interaction region.

In the $e^{+} e^{-}$channel, two electron candidates are required with transverse energy $E_{T}>25 \mathrm{GeV},|\eta|<2.47$; the region $1.37 \leqslant|\eta| \leqslant$ 1.52 is excluded because it corresponds to a transition region between the barrel and endcap calorimeters which has degraded energy resolution. Electron candidates are formed from clusters of cells reconstructed in the electromagnetic calorimeter. Criteria on the transverse shower shape, the longitudinal leakage into the hadronic calorimeter, and the association to an inner detector track are applied to the cluster to satisfy the Medium electron definition $[20,21]$. The electron energy is obtained from the calorimeter measurements and its direction from the associated track. A hit in the first layer of the pixel detector is required (if an active pixel layer is traversed) to suppress background from photon conversions. In addition, a fiducial cut removes events with electrons near problematic regions of the electromagnetic calorimeter during the 2010 run, reducing the acceptance by $6 \%$. The two electron candidates are not required to have opposite charge because of possible charge mis-identification either due to bremsstrahlung or to the limited momentum resolution of the inner detector at very high $p_{\mathrm{T}}$. For these selection criteria, the overall event acceptance for a $Z^{\prime} \rightarrow e^{+} e^{-}$of mass 1 TeV is $60 \%$.

In the $\mu^{+} \mu^{-}$channel, two muon candidates of opposite charge are required, each satisfying $p_{\mathrm{T}}>25 \mathrm{GeV}$. These muons are required to be within the trigger acceptance of $|\eta|<2.4$. Muon tracks are reconstructed independently in both the inner detector and muon spectrometer. The momentum is taken from a combined fit to the measurements from both subsystems. To obtain optimal momentum resolution, the muons used in this analysis are

[^10]required to have at least three hits in each of the inner, middle, and outer detectors of the muon system, and at least one hit in the non-bend plane. Residual misalignments of the muon detectors, which could cause a degradation of the momentum resolution, were studied with cosmic rays and with collision data in which the muons traversed overlapping sets of muon chambers. The effect of the misalignments, and the intrinsic position resolution, are included in the simulation and correspond to a resolution of $(20 \pm 4) \%$ for 1 TeV muons for the present data set. Studies of muons from $W$ decays verified that the observed momentum spectrum agrees with the simulation up to $p_{\mathrm{T}}=300 \mathrm{GeV}$ above which the event numbers are sparse. To suppress background from cosmic rays, the muons are also required to satisfy selections on the impact parameter, $\left|d_{0}\right|<0.2 \mathrm{~mm} ; z$ coordinate with respect to the primary vertex (PV), $\left|z_{0}-z(\mathrm{PV})\right|<1 \mathrm{~mm}$; and on the $z$ position of the primary vertex, $|z(\mathrm{PV})|<200 \mathrm{~mm}$. To reduce the background from jets, each muon is required to be isolated such that $\sum p_{\mathrm{T}}(\Delta R<0.3) / p_{\mathrm{T}}(\mu)<0.05$, where $\sum p_{\mathrm{T}}(\Delta R<0.3)$ is the sum of the $p_{\mathrm{T}}$ of the other tracks in a cone $\Delta R<0.3$ around the direction of the muon $\left(\Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \varphi)^{2}}\right)$. The overall event acceptance is $40 \%$ for a $Z^{\prime} \rightarrow \mu^{+} \mu^{-}$of mass 1 TeV . The primary reason for the lower acceptance compared to the electron channel is the requirement that hits are observed in all three layers of muon chambers, which reduces coverage in some regions of $\eta$. It is expected that this acceptance difference will be recovered in the future.

For both channels, the dominant background originates with the $Z / \gamma^{*}$ (Drell-Yan) process, which has the same final state as $Z^{\prime}$ or $Z^{*}$ production. In the $e^{+} e^{-}$channel, the second largest background arises from QCD jet production including $b$ quarks (referred to below as QCD background); above $m_{e^{+} e^{-}}=110 \mathrm{GeV}$, the next largest backgrounds are $t \bar{t}$ and $W+$ jets events. In the $\mu^{+} \mu^{-}$channel, in order of dominance the backgrounds are Drell-Yan production, followed by $t \bar{t}$ and diboson ( $W W, W Z$ and $Z Z$ ) production; the QCD and $W+$ jets backgrounds are negligible.

Expected signal and backgrounds, with the exception of the QCD component, are evaluated with simulated samples and normalized with respect to one another using the highest-order available cross section predictions. The $Z^{\prime}$ signal and $Z / \gamma^{*}$ processes are generated with PYthia 6.421 [22] using MRST2007 LO* [23] parton distribution functions (PDFs). The $Z_{S S M}^{\prime}$ was used as the benchmark signal model and this signal sample was generated with Pythia using Standard Model couplings. $Z^{*}$ events are generated with CompHEP [24] using CTEQ6L1 [25] PDFs followed by Pythia for parton showering and underlying event generation. The diboson processes are generated with Herwig 6.510 [26,27] using MRST2007 LO* PDFs. The $W+$ jets background is generated with Alpgen [28] and the $t \bar{t}$ background with MC@NLO 3.41 [29]. For both, Jimmy 4.31 [30] is used to describe multiple parton interactions and Herwig to describe the remaining underlying event and parton showers. CTEQ [25] parton distribution functions are used. For all samples, final state photon radiation is handled by Рнотоs [31] and the interaction of particles and the response of the detector are carried out using full detector simulation [32] based on Geant4 [33].

The $Z / \gamma^{*}$ cross section is calculated at next-to-next-to-leading order (NNLO) using PHOZPR [34] with MSTW2008 parton distribution functions [35]. The ratio of this cross section to the leadingorder cross section can be used to determine a mass dependent QCD K-factor which is applied to the results of the leading-order simulations. The same QCD K-factor is applied to the $Z^{\prime}$ signal. However, the QCD K-factor is not applied to the leading-order $Z^{*}$ cross section since the $Z^{*}$ model uses an effective Lagrangian with a different Lorentz structure. Higher-order weak corrections (beyond the photon radiation included in the simulation) are
calculated using HORACE $[36,37]$, yielding a weak K-factor due to virtual heavy gauge boson loops. The weak K-factor is not applied to the $Z^{\prime}$ or $Z^{*}$ signal since it is not universal, but depends on the coupling of the $W$ and $Z$ bosons to the $Z^{\prime}$ or $Z^{*}$. The diboson cross section is known to next-to-leading order (NLO) with an uncertainty of $5 \%$. The $W+$ jets cross section is calculated at NLO, and rescaled to the inclusive NNLO calculation, resulting in $30 \%$ uncertainty when at least one parton with $E_{T}>20 \mathrm{GeV}$ accompanies the $W$ boson. The $t \bar{t}$ cross section is predicted at approximate-NNLO, with $10 \%$ uncertainty [38-40]. Cross section uncertainties are estimated from PDF error sets and from variation of renormalization and factorization scales in the cross section calculation.

To estimate the QCD background in the $e^{+} e^{-}$sample, a combination of three different techniques is used. In the "reversed electron identification" technique, a sample of events where both electrons pass the Loose electron identification selections [20,21] but fail the Medium selections is used to determine the shape of the QCD background as a function of invariant mass $m_{e^{+}} e^{-}$. This template shape, and the sum of the Drell-Yan, diboson, $t \bar{t}$ and $W+$ jets backgrounds, are fitted to the observed $m_{e^{+} e^{-}}$distribution to determine the normalization of the QCD contribution. In the second technique [21], the isolation distribution for the electrons (energy in the calorimeter in a cone of $\Delta R<0.4$ around the electron track after subtracting the electron cluster energy) is fitted to a signal template, corresponding to electrons from either $Z$ or $Z^{\prime} \mid Z^{*}$ production, plus a background template; the latter is determined from the data by reversing electron identification selections. The third technique relates, via a matrix inversion, the measured number of events passing Loose or Medium, plus first-pixel-layer hit, identification requirements for each of the two electrons (i.e. four different categories of events) to the true number of real and fake electron combinations in the sample [41,42]. To combine the measurements from each of these estimates and obtain the QCD background in the high $-m_{e^{+} e^{-}}$region, a fit in several bins of $m_{e^{+}} e^{-}$above 110 GeV is performed using a power-law function of $m_{e^{+} e^{-}}$with the parameters being the exponent and the integral number of events with $m_{e^{+} e^{-}}>110 \mathrm{GeV}$. The background in any given region of $m_{e^{+} e^{-}}$is then obtained from an integral of this function; the corresponding uncertainty is obtained by propagating the statistical and systematic uncertainties for each of the background estimation methods. A small additional systematic uncertainty related to a small bias in the fit for low statistics and variations when different functions were used is also taken into account. The power law function gives a conservative estimate of the QCD background at very large $m_{e^{+} e^{-}}$, as it falls less rapidly than other functional forms used to fit dijet invariant mass distributions [43].

QCD backgrounds in the $\mu^{+} \mu^{-}$sample can be produced by pion and kaon decay in flight or from semi-leptonic decays of $b$ and $c$ quarks. The former is suppressed by the small decay probability of a high- $p_{\mathrm{T}}$ pion or kaon. The background from semi-leptonic decays of $b$ and $c$ quarks is evaluated using the $\sum_{B D} p_{\mathrm{T}}(\Delta R<0.3) / p_{\mathrm{T}}(\mu)$ isolation variable. A simulated sample of $b \bar{b}$ and $c \bar{c}$ events is shown to reproduce the isolation distribution of the muon candidates, after all selection cuts except isolation are applied. This simulated QCD sample is normalized to the data in the region $\sum p_{\mathrm{T}}(\Delta R<0.3) / p_{\mathrm{T}}(\mu)>0.1$, and then used to predict the background passing the final selection criterion of $\sum p_{\mathrm{T}}(\Delta R<0.3) / p_{\mathrm{T}}(\mu)<0.05$. A systematic uncertainty of $50 \%$ is assigned to the QCD background to cover the difference between the number of non-isolated muons predicted by the simulation and the number observed in the data.

A direct estimate of background from cosmic rays in the muon channel is obtained by observing the rate, and mass distribution, of


Fig. 1. Dielectron invariant mass ( $m_{e^{+} e^{-}}$) distribution after final selection, compared to the stacked sum of all expected backgrounds, with three example $Z_{\text {SSM }}^{\prime}$ signals overlaid. The bin width is constant in $\log m_{e^{+} e^{-}}$and the ratio of the upper to lower bounds of each bin is 1.07 .
events satisfying $3<\left|z_{0}-z(\mathrm{PV})\right|<200 \mathrm{~mm}$ or $\left|d_{0}\right|>0.3 \mathrm{~mm}$. The number of events in the final sample is obtained by scaling to the number expected to pass the $\left|d_{0}\right|<0.2 \mathrm{~mm}$, and $\left|z_{0}-z(\mathrm{PV})\right|<$ 1 mm selection criteria. The total cosmic ray background above $m_{\mu^{+} \mu^{-}}=70 \mathrm{GeV}$ is thus estimated to be $0.004 \pm 0.002$ events.

Finally, while the primary estimate of the $t \bar{t}$ background is taken from Monte Carlo for both channels as discussed above, a data-driven cross-check of the $t \bar{t}$ background was also performed. The $e \mu$ final state with dilepton invariant mass $>100 \mathrm{GeV}$ provides an enriched sample of $t \bar{t}$ fully leptonic events. After correcting for relative efficiencies, it provides a direct estimate from data of the $t \bar{t} \rightarrow e^{+} e^{-}, \mu^{+} \mu^{-}$backgrounds. The results, which have relatively large statistical uncertainties due to the limited number of events, are in good agreement with the Monte Carlo prediction.

The observed invariant mass distributions, $m_{e^{+} e^{-}}$and $m_{\mu^{+} \mu^{-}}$, are compared to the expectation of the SM backgrounds. To make this comparison, the sum of the Drell-Yan, $t \bar{t}$, diboson and $W+$ jets backgrounds (with the relative contributions fixed according to the respective cross sections) is scaled such that when added to the data-driven QCD background, the result agrees with the observed number of data events in the $70-110 \mathrm{GeV}$ mass interval. The advantage of this approach is that the uncertainty on the luminosity, and any mass independent uncertainties in efficiencies, cancel between the $Z^{\prime} \mid Z^{*}$ and the $Z$ in the limit computation presented below. The integrated Drell-Yan cross section at NNLO above a generator-level dilepton invariant mass of 60 GeV is ( $0.989 \pm 0.049$ ) nb.

Fig. 1 presents the invariant mass ( $m_{e^{+} e^{-}}$) distribution after final selection while Table 1 shows the number of data events and estimated backgrounds in bins of reconstructed $e^{+} e^{-}$invariant mass. The dielectron invariant mass distribution is well described by the prediction from SM processes.

Similarly, Fig. 2, and Table 2 show the results for the $\mu^{+} \mu^{-}$ sample. Again, there is good agreement with the prediction from SM processes. Figs. 1 and 2 also display expected $Z_{\text {SSM }}^{\prime}$ signals for three masses around 1 TeV . Expected $Z^{*}$ signals (not shown) have a similar shape and approximately $40 \%$ higher cross section. Three events in the vicinity of $m_{e^{+} e^{-}}=600 \mathrm{GeV}$ and a single event at $m_{\mu^{+} \mu^{-}}=768 \mathrm{GeV}$ are observed in the data. The $p$-value which quantifies, in the absence of signal, the probability of observing an excess anywhere in the search region $m_{\ell^{+} \ell^{-}}>110 \mathrm{GeV}(\ell=e$ or $\mu$ ), with a significance at least as great as that observed in the

Table 1
 are correlated across bins and are discussed in the text. Entries of 0.0 indicate a value $<0.05$.

| $m_{e^{+} e^{-}}[\mathrm{GeV}]$ | 70-110 | 110-130 | 130-150 | 150-170 | 170-200 | 200-240 | 240-300 | 300-400 | 400-800 | 800-2000 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $Z / \gamma^{*}$ | $8498.5 \pm 7.9$ | $104.9 \pm 3.3$ | $36.8 \pm 1.3$ | $19.4 \pm 0.7$ | $14.7 \pm 0.6$ | $9.5 \pm 0.4$ | $6.0 \pm 0.3$ | $3.2 \pm 0.1$ | $1.6 \pm 0.1$ | $0.1 \pm 0.0$ |
| $t \bar{t}$ | $8.2 \pm 0.8$ | $2.8 \pm 0.3$ | $2.1 \pm 0.2$ | $1.7 \pm 0.2$ | $1.7 \pm 0.2$ | $1.2 \pm 0.1$ | $0.9 \pm 0.1$ | $0.5 \pm 0.0$ | $0.2 \pm 0.0$ | $0.0 \pm 0.0$ |
| Diboson | $12.1 \pm 0.9$ | $1.0 \pm 0.2$ | $0.7 \pm 0.2$ | $0.5 \pm 0.2$ | $0.5 \pm 0.1$ | $0.4 \pm 0.1$ | $0.3 \pm 0.1$ | $0.2 \pm 0.1$ | $0.1 \pm 0.1$ | $0.0 \pm 0.0$ |
| $W+$ jets | $6.0 \pm 1.8$ | $3.7 \pm 1.2$ | $1.2 \pm 0.5$ | $1.3 \pm 0.5$ | $1.2 \pm 0.4$ | $1.1 \pm 0.4$ | $0.3 \pm 0.1$ | $0.2 \pm 0.1$ | $0.2 \pm 0.1$ | $0.0 \pm 0.0$ |
| QCD | $32.1 \pm 7.1$ | $8.4 \pm 1.8$ | $5.5 \pm 0.8$ | $3.2 \pm 0.6$ | $2.8 \pm 0.8$ | $1.9 \pm 0.8$ | $1.3 \pm 0.7$ | $0.8 \pm 0.4$ | $0.5 \pm 0.2$ | $0.1 \pm 0.1$ |
| Total | $8557.0 \pm 10.8$ | $120.9 \pm 4.0$ | $46.4 \pm 1.6$ | $26.2 \pm 1.1$ | $20.8 \pm 1.1$ | $14.1 \pm 1.0$ | $8.8 \pm 0.7$ | $4.8 \pm 0.5$ | $2.7 \pm 0.3$ | $0.2 \pm 0.1$ |
| Data | 8557 | 131 | 49 | 20 | 18 | 13 | 9 | 3 | 3 | 0 |

Table 2
 are correlated across bins and are discussed in the text. Entries of 0.0 indicate a value $<0.05$.

| $m_{\mu^{+} \mu^{-}}[\mathrm{GeV}]$ | 70-110 | 110-130 | 130-150 | 150-170 | 170-200 | 200-240 | 240-300 | 300-400 | 400-800 | 800-2000 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $Z / \gamma^{*}$ | $7546.7 \pm 7.1$ | $98.4 \pm 3.1$ | $33.4 \pm 1.1$ | $17.2 \pm 0.6$ | $12.8 \pm 0.5$ | $7.8 \pm 0.3$ | $5.1 \pm 0.2$ | $2.5 \pm 0.1$ | $1.3 \pm 0.1$ | $0.1 \pm 0.0$ |
| $t \bar{t}$ | $6.0 \pm 0.6$ | $2.4 \pm 0.3$ | $1.7 \pm 0.2$ | $1.2 \pm 0.1$ | $1.2 \pm 0.1$ | $1.0 \pm 0.1$ | $0.7 \pm 0.1$ | $0.4 \pm 0.0$ | $0.1 \pm 0.0$ | $0.0 \pm 0.0$ |
| Diboson | $10.0 \pm 0.5$ | $0.8 \pm 0.1$ | $0.6 \pm 0.0$ | $0.5 \pm 0.0$ | $0.4 \pm 0.0$ | $0.3 \pm 0.0$ | $0.2 \pm 0.0$ | $0.2 \pm 0.0$ | $0.1 \pm 0.0$ | $0.0 \pm 0.0$ |
| $W+$ jets | $0.3 \pm 0.2$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ |
| QCD | $0.1 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ | $0.0 \pm 0.0$ |
| Total | $7563.0 \pm 7.2$ | $101.6 \pm 3.1$ | $35.7 \pm 1.2$ | $18.9 \pm 0.7$ | $14.4 \pm 0.5$ | $9.1 \pm 0.4$ | $6.0 \pm 0.2$ | $3.0 \pm 0.1$ | $1.5 \pm 0.1$ | $0.1 \pm 0.0$ |
| Data | 7563 | 101 | 41 | 11 | 11 | 7 | 6 | 2 | 1 | 0 |



Fig. 2. Dimuon invariant mass ( $m_{\mu^{+} \mu^{-}}$) distribution after final selection, compared to the stacked sum of all expected backgrounds, with three example $Z_{\text {SSM }}^{\prime}$ signals overlaid. The bin width is constant in $\log m_{\mu^{+} \mu^{-}}$and the ratio of the upper to lower bounds of each bin is 1.07 .
data is evaluated [44]. Since the resulting $p$-values are $5 \%$ and $22 \%$ for the electron and muon channels, respectively, no statistically significant excess above the predictions of the SM has been observed.

Given the absence of a signal, an upper limit on the number of $Z^{\prime}$ events is determined at the $95 \%$ confidence level (C.L.) using a Bayesian approach [44]. The invariant mass distribution of the data is compared to templates of the expected backgrounds and varying amounts of signal at varying pole masses in the 0.132.0 TeV range, a technique used in Ref. [45]. A likelihood function is defined as the product of the Poisson probabilities over all mass bins in the search region, where the Poisson probability in each bin is evaluated for the observed number of data events given the expectation from the template. The total acceptance for signal as a function of mass is propagated into the expectation. For each $Z^{\prime}$ pole mass, a uniform prior in the $Z^{\prime}$ cross section is used.

The normalization procedure described above makes this analysis insensitive to the uncertainty on the integrated luminosity as well as other mass-independent systematic uncertainties. Massdependent systematic uncertainties are incorporated as nuisance parameters whose variation is integrated over in the computation of the likelihood function [44]. The relevant systematic uncertainties are reconstruction efficiency, QCD and weak K-factors, PDF and resolution uncertainties. These uncertainties are correlated across all bins in the search region, and they are correlated between signal and background except for the weak K-factor which is only applied to the Drell-Yan background. In addition, there is an uncertainty on the QCD component of the background for the electron channel.

The uncertainties on the mass-dependent nuisance parameters are as follows: since the total background is normalized to the data in the region of the $Z \rightarrow \ell^{+} \ell^{-}$mass peak, the residual systematic uncertainties are small at low mass and grow at high mass. The dominant uncertainties are of a theoretical nature. The uncertainty on the cross sections due to PDF variation is $6 \%(8 \%)$ at 1 TeV for $Z^{\prime}$ $\left(Z^{*}\right)$ production, for both channels. The uncertainties on the QCD and weak K-factors are $3 \%$ and $4.5 \%$ respectively for both channels. The uncertainty in the weak K-factor includes the effects of neglecting real boson emission, the difference in the electroweak scheme definition between Pythia and horace, and higher-order electroweak and $\mathcal{O}\left(\alpha \alpha_{s}\right)$ corrections. Finally, an uncertainty of $5 \%$, due to the uncertainty on the $Z / \gamma^{*}$ cross section in the normalization region, as well as a $1 \%$ statistical error on the data in the normalization region, are applied.

On the experimental side, the systematic effects are as follows. In the electron channel, the calorimeter resolution is dominated at large transverse energy by a constant term which is $1.1 \%$ in the barrel and $1.8 \%$ in the endcaps with a small uncertainty. The simulation was adjusted to reproduce this resolution at high energy and the uncertainty on it has a negligible effect. The calorimeter energy calibration uncertainty is between $0.5 \%$ and $1.5 \%$ depending on transverse momentum and pseudorapidity. The non-linearity of the calorimeter response is negligible according to test beam data and Monte Carlo studies [46]. The uncertainty on the energy calibration has minimal impact on the sensitivity of the search,

Table 3
Summary of systematic uncertainties on the expected numbers of events at $m_{\ell^{+} \ell^{-}}=1 \mathrm{TeV}$. NA indicates that the uncertainty is not applicable, and "-" denotes a negligible entry.

| Source | Dielectrons |  |  | Dimuons |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  | $Z^{\prime}$ signal | background |  | $Z^{\prime}$ signal | background |
| Normalization | $5 \%$ | $5 \%$ |  | $5 \%$ | $5 \%$ |
| PDFs | $6 \%$ | $6 \%$ |  | $6 \%$ | $6 \%$ |
| QCD K-factor | $3 \%$ | $3 \%$ | $3 \%$ | $3 \%$ |  |
| Weak K-factor | NA | $4.5 \%$ |  | NA | $4.5 \%$ |
| Efficiency | - | - | $3 \%$ | $3 \%$ |  |
| Resolution | - | - | $3 \%$ | $3 \%$ |  |
| Total | $9.4 \%$ | $9.5 \%$ |  | $9.4 \%$ | $10.4 \%$ |

since its main effect is a shift of a potential peak in dilepton mass without change of the line-shape. No source of efficiency variation for electron reconstruction and identification at high $p_{\mathrm{T}}$ has been found.

For the muon channel, the combined uncertainty on the trigger and reconstruction efficiency is estimated to be $3 \%$ at 1 TeV . This uncertainty is dominated by the rate of muon bremsstrahlung in the calorimeter which may interfere with reconstruction in the muon spectrometer. The uncertainty on the resolution due to residual misalignments in the muon spectrometer propagates to a change in the observed width of $Z^{\prime} \mid Z^{*}$ line-shape, and affects the sensitivity by $3 \%$. The muon momentum scale is calibrated with a statistical precision of $0.2 \%$ using the $Z \rightarrow \ell^{+} \ell^{-}$mass peak. As with the electron channel, the momentum calibration uncertainty has negligible impact in the muon channel search. The systematic uncertainties are summarized in Table 3.

The limit on the number of $Z^{\prime}$ events produced is converted into a limit on cross section times branching ratio $\sigma B\left(Z^{\prime} \rightarrow \ell^{+} \ell^{-}\right)$ by scaling with the observed number of $Z$ boson events and the known value of $\sigma B\left(Z \rightarrow \ell^{+} \ell^{-}\right)$. The expected exclusion limits are determined using simulated pseudo-experiments containing only Standard Model processes by evaluating the $95 \%$ C.L. upper limits for each pseudo-experiment for each fixed value of $M_{Z^{\prime}}$. The median of the distribution of limits is chosen to represent the expected limit. The ensemble of limits is also used to find the $68 \%$ and $95 \%$ envelope of the expected limits as a function of $M_{Z^{\prime}}$.

Fig. 3 shows for the dielectron channel the 95\% C.L. observed and expected exclusion limits on $\sigma B$. It also shows the theoretical cross section times branching ratio for the $Z_{S S M}^{\prime}$ and for the lowest and highest $\sigma B$ of $E_{6}$-motivated $Z^{\prime}$ models. Similarly, Fig. 4 shows the same results in the case of the dimuon channel. Fig. 5 shows the $95 \%$ C.L. exclusion limit on $\sigma B$ for the combination of the electron and muon channels. The combination is performed by defining the likelihood function in terms of the total number of $Z^{\prime}$ events produced in both channels.

In the three cases (dielectron, dimuon and combined channels), the $95 \%$ C.L. $\sigma B$ limit is used to set mass limits for each of the considered models. Mass limits obtained for the $Z_{\text {SSM }}^{\prime}$ are displayed in Table 4 together with the corresponding $\sigma B$ limit. The combined mass limit for the $Z_{\text {SSM }}^{\prime}$ is 1.048 TeV (observed) and 1.088 TeV (expected). The combined mass limits on the $E_{6}$-motivated models are given in Table 5. The limits on the $E_{6}$-motivated $Z_{I}^{\prime}$ and $Z_{S}^{\prime}$ are 0.842 TeV and 0.871 TeV , more stringent than the previous highest limits [18].

Although the lepton decay angular distributions are not the same for $Z^{\prime}$ and $Z^{*}$ bosons, we found the difference in geometrical acceptance to be negligible for boson pole masses above 750 GeV . The same procedure as for the $Z^{\prime}$ is used to calculate a limit on $\sigma B\left(Z^{*} \rightarrow \ell^{+} \ell^{-}\right)$and on the $Z^{*}$ mass in each channel and for their combination. The results are displayed in Table 6. The combined


Fig. 3. Expected and observed $95 \%$ C.L. limits on $\sigma B$ and expected $\sigma B$ for $Z_{\mathrm{SSM}}^{\prime}$ production and the two $E_{6}$-motivated $Z^{\prime}$ models with lowest and highest $\sigma B$ for the dielectron channel. The thickness of the SSM theory curve represents the theoretical uncertainty and holds for the other theory curves.


Fig. 4. Expected and observed $95 \%$ C.L. limits on $\sigma B$ and expected $\sigma B$ for $Z_{S S M}^{\prime}$ production and the two $E_{6}$-motivated $Z^{\prime}$ models with lowest and highest $\sigma B$ for the dimuon channel. The thickness of the SSM theory curve represents the theoretical uncertainty and holds for the other theory curves.


Fig. 5. Expected and observed $95 \%$ C.L. limits on $\sigma B$ and expected $\sigma B$ for $Z_{\text {SSM }}^{\prime}$ production and the two $E_{6}$-motivated $Z^{\prime}$ models with lowest and highest $\sigma B$ for the combination of the electron and muon channels. The thickness of the $Z_{S S M}^{\prime}$ theory curve represents the theoretical uncertainty and holds for the other theory curves.

Table 4
$e^{+} e^{-}, \mu^{+} \mu^{-}$and combined $95 \%$ C.L. mass and $\sigma B$ limits on $Z_{\text {SSM }}^{\prime}$.

|  | Observed limit |  |  | Expected limit |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  | mass [TeV] | $\sigma B[\mathrm{pb}]$ |  | mass [TeV] | $\sigma B[\mathrm{pb}]$ |
| $Z_{\text {SSM }}^{\prime} \rightarrow e^{+} e^{-}$ | 0.957 | 0.155 |  | 0.967 | 0.145 |
| $Z_{\text {SSM }}^{\prime} \rightarrow \mu^{+} \mu^{-}$ | 0.834 | 0.297 |  | 0.900 | 0.201 |
| $Z_{\text {SSM }}^{\prime} \rightarrow \ell^{+} \ell^{-}$ | 1.048 | 0.094 |  | 1.088 | 0.081 |

Table 5
Combined mass limits at $95 \%$ C.L. on the $E_{6}$-motivated $Z^{\prime}$ models.

| Model | $Z_{\psi}^{\prime}$ | $Z_{\mathrm{N}}^{\prime}$ | $Z_{\eta}^{\prime}$ | $Z_{I}^{\prime}$ | $Z_{\mathrm{S}}^{\prime}$ | $Z_{\chi}^{\prime}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Mass limit $[\mathrm{TeV}]$ | 0.738 | 0.763 | 0.771 | 0.842 | 0.871 | 0.900 |

## Table 6

$e^{+} e^{-}, \mu^{+} \mu^{-}$and combined $95 \%$ C.L. mass and $\sigma B$ limits on $Z^{*}$ production.

|  | Observed limit |  |  |  | Expected limit |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :---: |
|  | mass $[\mathrm{TeV}]$ | $\sigma B[\mathrm{pb}]$ |  | mass $[\mathrm{TeV}]$ | $\sigma B[\mathrm{pb}]$ |  |
| $Z^{*} \rightarrow e^{+} e^{-}$ | 1.058 | 0.149 |  | 1.062 | 0.143 |  |
| $Z^{*} \rightarrow \mu^{+} \mu^{-}$ | 0.946 | 0.265 |  | 0.995 | 0.199 |  |
| $Z^{*} \rightarrow \ell^{+} \ell^{-}$ | 1.152 | 0.089 |  | 1.185 | 0.080 |  |

mass limit for the $Z^{*}$ boson is 1.152 TeV (observed) and 1.185 TeV (expected). This is the first direct limit on this particle.

In conclusion, the ATLAS detector has been used to search for narrow resonances in the invariant mass spectrum above 110 GeV of $e^{+} e^{-}$and $\mu^{+} \mu^{-}$final states with $\sim 40 \mathrm{pb}^{-1}$ of proton-proton data. No evidence for such a resonance is found. Limits on the cross section times branching ratio $\sigma B\left(Z^{\prime} \rightarrow \ell^{+} \ell^{-}\right)$are calculated, as well as mass limits on the $Z_{\text {SSM }}^{\prime}(1.048 \mathrm{TeV})$, the $Z^{*}(1.152 \mathrm{TeV})$ and $E_{6}$-motivated $Z^{\prime}$ bosons (in the range $0.738-0.900 \mathrm{TeV}$ ). For certain $E_{6}$-motivated models, these limits are more stringent than the corresponding limits from the Tevatron.

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E. Katsoufis ${ }^{9}$, J. Katzy ${ }^{41}$, V. Kaushik ${ }^{6}$, K. Kawagoe ${ }^{67}$, T. Kawamoto ${ }^{155}$, G. Kawamura ${ }^{81}$, M.S. Kayl ${ }^{105}$, V.A. Kazanin ${ }^{107}$, M.Y. Kazarinov ${ }^{65}$, S.I. Kazi ${ }^{86}$, J.R. Keates ${ }^{82}$, R. Keeler ${ }^{169}$, R. Kehoe ${ }^{39}$, M. Keil ${ }^{54}$, G.D. Kekelidze ${ }^{65}$, M. Kelly ${ }^{82}$, J. Kennedy ${ }^{98}$, C.J. Kenney ${ }^{143}$, M. Kenyon ${ }^{53}$, O. Kepka ${ }^{125}$, N. Kerschen ${ }^{29}$, B.P. Kerševan ${ }^{74}$, S. Kersten ${ }^{174}$, K. Kessoku ${ }^{155}$, C. Ketterer ${ }^{48}$, M. Khakzad ${ }^{28}$, F. Khalil-zada ${ }^{10}$, H. Khandanyan ${ }^{165}$, A. Khanov ${ }^{112}$, D. Kharchenko ${ }^{65}$, A. Khodinov ${ }^{148}$, A.G. Kholodenko ${ }^{128}$, A. Khomich ${ }^{58 a}$, T.J. Khoo ${ }^{27}$, G. Khoriauli ${ }^{20}$, N. Khovanskiy ${ }^{65}$, V. Khovanskiy ${ }^{95}$, E. Khramov ${ }^{65}$, J. Khubua ${ }^{51}$, G. Kilvington ${ }^{\text {6 }}$, H. Kim ${ }^{7}$, M.S. 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# Search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ with the ATLAS detector ${ }^{\text {* }}$ 

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#### Abstract

A search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{\prime+} \ell^{\prime-}$, where $\ell=e, \mu$, is presented. Proton-proton collision data at $\sqrt{s}=7 \mathrm{TeV}$ recorded with the ATLAS detector and corresponding to an average integrated luminosity of $2.1 \mathrm{fb}^{-1}$ are compared to the Standard Model expectations. Upper limits on the production cross section of a Standard Model Higgs boson with a mass between 110 and 600 GeV are derived. The observed (expected) $95 \%$ confidence level upper limit on the production cross section for a Higgs boson with a mass of 194 GeV , the region with the best expected sensitivity for this search, is 0.99 (1.01) times the Standard Model prediction. The Standard Model Higgs boson is excluded at $95 \%$ confidence level in the mass ranges 191-197, 199-200 and 214-224 GeV.


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## 1. Introduction

The search for the Standard Model (SM) Higgs boson [1-3] is a major goal of the Large Hadron Collider (LHC) programme. Direct searches at the CERN LEP $e^{+} e^{-}$collider led to a lower limit on the Higgs boson mass, $m_{H}$, of 114.4 GeV at $95 \%$ confidence level (CL) [4]. The searches at the Fermilab Tevatron $p \bar{p}$ collider have excluded at $95 \% \mathrm{CL}$ the region $156 \mathrm{GeV}<m_{H}<$ 177 GeV [5]. Results from the 2010 LHC run extended the search in the region $200 \mathrm{GeV}<m_{H}<600 \mathrm{GeV}$ by excluding a Higgs boson with cross section larger than 5-20 times the SM prediction [6,7].

This Letter presents a search for the SM Higgs boson in the mass range from 110 to 600 GeV in the channel $H \rightarrow$ $Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{\prime+} \ell^{\prime-}$, where $\ell, \ell^{\prime}=e, \mu$. Three distinct final states, $\mu \mu \mu \mu(4 \mu)$, ее $\mu \mu(2 e 2 \mu)$, and eeee ( $4 e$ ), are selected. The largest background to this search comes from continuum $Z Z^{(*)}$ production. For $m_{H}<180 \mathrm{GeV}$, contributions from $Z+$ jets and $t \bar{t}$ processes, where the additional charged leptons arise either from semi-leptonic decays of heavy flavour or from light flavour jets misidentified as leptons, are important. The $p p$ collision data were recorded with the ATLAS detector at the LHC at $\sqrt{s}=7 \mathrm{TeV}$ and correspond to an average integrated luminosity of $2.1 \mathrm{fb}^{-1}$ [8].

[^12]
## 2. The ATLAS detector

The ATLAS detector [9] is a multi-purpose particle physics apparatus with forward-backward symmetric cylindrical geometry. ${ }^{1}$ The inner tracking detector (ID) consists of a silicon pixel detector, a silicon microstrip detector, and a transition radiation tracker. The ID is surrounded by a thin superconducting solenoid providing a 2 T magnetic field. A high-granularity lead-liquid argon (LAr) sampling calorimeter measures the energy and the position of electromagnetic showers. An iron-scintillator tile calorimeter provides hadronic coverage in the central rapidity range. The end-cap and forward rapidity regions are instrumented with LAr calorimetry for both electromagnetic and hadronic measurements. The muon spectrometer (MS) surrounds the calorimeters and consists of three large superconducting toroids, each with eight coils, a system of precision tracking chambers, and detectors for triggering. A threelevel trigger system selects events to be recorded for offline analysis.

## 3. Data and simulation samples

The accumulated data are subjected to quality requirements ensuring that the relevant detector components were operating

[^13]Table 1
Higgs boson production cross sections for both gluon and vector-boson fusion processes in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$. The cross sections include the branching ratio of $H \rightarrow 4 \ell$, with $\ell=e, \mu$. The errors are the total theoretical systematic uncertainty.

| $m_{H}$ <br> $[\mathrm{GeV}]$ | $\sigma(g g \rightarrow H)$ <br> $[\mathrm{pb}]$ | $\sigma(q q \rightarrow H)$ <br> $[\mathrm{pb}]$ | $\mathrm{BR}(H \rightarrow 4 \ell)$ <br> $\cdot 10^{-3}$ |
| :--- | :--- | :--- | :--- |
| 130 | $14.1_{-2.1}^{+2.7}$ | $1.154_{-0.027}^{+0.032}$ | 0.19 |
| 150 | $10.5_{-1.6}^{+2.0}$ | $0.962_{-0.021}^{+0.028}$ | 0.38 |
| 200 | $5.2_{-0.8}^{+0.9}$ | $0.637_{-0.015}^{+0.022}$ | 1.15 |
| 240 | $3.6 \pm 0.6$ | $0.464_{-0.012}^{+0.018}$ | 1.32 |
| 300 | $2.4 \pm 0.3$ | $0.301_{-0.008}^{+0.014}$ | 1.38 |
| 400 | $2.0 \pm 0.3$ | $0.162_{-0.005}^{+0.010}$ | 1.21 |
| 600 | $0.33 \pm 0.06$ | $0.058_{-0.002}^{+0.005}$ | 1.23 |

normally. The resulting average integrated luminosity of $2.1 \mathrm{fb}^{-1}$ corresponds to $2.28 \mathrm{fb}^{-1}, 1.96 \mathrm{fb}^{-1}$ and $1.98 \mathrm{fb}^{-1}$ for the $4 \mu$, $2 e 2 \mu$ and $4 e$ final states, respectively.

The $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ signal is modelled using the powheg Monte Carlo (MC) event generator [10,11], which calculates separately the gluon and vector-boson fusion production mechanisms with matrix elements up to next-to-leading order (NLO). The Higgs boson transverse momentum, $p_{\mathrm{T}}$, spectrum is reweighted to the calculation of Ref. [12], providing QCD corrections up to next-to-leading order and QCD soft-gluon resummations up next-to-next-to-leading log (NNLL). powheg is interfaced to pythia [13] for showering and hadronization, which in turn is interfaced to рнотоs [14] for QED radiative corrections in the final state and to tauola [ 15,16 ] for the simulation of $\tau$ decays.

The cross sections for Higgs boson production, the corresponding branching fractions, as well as their uncertainties [17], are derived to next-to-next-to-leading order (NNLO) in QCD for the gluon fusion [18-23] and vector-boson fusion [24] processes. In addition, QCD soft-gluon resummations up to NNLL are available for the gluon fusion process [25], while the NLO electroweak (EW) corrections are applied to both the gluon fusion [26,27] and vectorboson fusion [28,29] processes. The Higgs boson decay branching ratio to the four-lepton final state is predicted by prophecy 4 F [30, 31], which includes the complete NLO QCD + EW corrections, interference effects between identical final state fermions and leading two-loop heavy Higgs boson corrections to the four-fermion width. Table 1 gives the production cross sections for the $H \rightarrow 4 \ell$ for several Higgs boson masses.

The $Z Z^{(*)}$ background is generated using PYTHIA, taking into account $Z-\gamma$ interference. For the inclusive total cross section and the shape of the $m_{Z Z^{(*)}}$ spectrum, the MCFM $[32,33]$ prediction is used, which includes both quark-antiquark annihilation at QCD NLO and gluon fusion. The inclusive $Z$ boson production, $Z+$ jets, is modelled using alpgen [34] and is divided into $Z+$ light flavour jets and $Z b \bar{b}$; overlaps between the two samples are removed. Specifically, $b \bar{b}$ pairs with separation $\Delta R=\sqrt{\Delta \phi^{2}+\Delta \eta^{2}} \geqslant 0.4$ between the $b$-jets are taken from the matrix-element calculation, whereas for $\Delta R<0.4$ the parton-shower jets are taken. PYTHIA is also used as a cross-check of the alpgen results. In this search the $Z+$ jets production is normalized from the data, but for comparisons the QCD NNLO FEWZ [35,36] and the MCFM $[32,33]$ cross section calculations are used for the inclusive $Z$ boson and the $Z b \bar{b}$ production, respectively. The $t \bar{t}$ background is modelled using mC@ NLO [37] and is normalized to the approximately NNLO cross section calculated using hathor [38]. Both Alpgen and mc@ NLo are interfaced to Herwig [39] for parton shower hadronization and to jimmy [40] for the underlying event simulations.

All generated events undergo a full detector simulation performed using GEANT4 [41,42].

The number of $p p$ interactions in the same bunch crossing (pileup) is included in the simulation. The MC samples are reweighted to reproduce the observed distribution in the data.

## 4. Physics object identification and event selection

The data considered in this analysis were selected using singlelepton triggers. For electrons the threshold on the transverse energy, $E_{T}$, was $20-22 \mathrm{GeV}$ depending on the LHC instantaneous luminosity and for muons the threshold on $p_{\mathrm{T}}$ was 18 GeV . Both triggers are more than $99.5 \%$ efficient for events passing the offline selection described below.

Electron candidates consist of clusters of energy deposited in the electromagnetic calorimeter associated to ID tracks. The electrons must satisfy the "medium" electron criteria [43], which require the shower profiles to be consistent with those expected for electromagnetic showers and a well reconstructed ID track pointing to the corresponding cluster. The electron transverse momentum is computed from the cluster energy and the track direction.

Muon candidates are reconstructed by matching ID tracks with either full or partial tracks in the MS [43]. For the former case, the two independent momentum measurements are combined, whereas for the latter case the momentum is measured using the ID information only, with the MS providing muon identification. To reject cosmic rays, tracks are required to be consistent with having originated from the primary vertex, defined as the reconstructed vertex with the highest $\sum p_{\mathrm{T}}^{2}$ of associated tracks.

Leptons from Higgs boson decays are expected to be isolated and to originate from a common vertex. Track and calorimeter isolation as well as transverse impact parameter significance requirements are therefore applied to further reduce the $Z+$ jets and $t \bar{t}$ contributions. The sum of $p_{\mathrm{T}}$ of tracks within $\Delta R<0.2$ of the lepton divided by the lepton $p_{\mathrm{T}}$ is required to be less than 0.15 , while the sum $E_{\mathrm{T}}$ of the calorimeter cells within $\Delta R<0.2$ around the lepton divided by the lepton $p_{T}$ is required to be less than 0.3 . In the case of electrons, the calorimeter cells corresponding to the electromagnetic shower are subtracted. The transverse impact parameter significance, defined as the transverse impact parameter of the lepton with respect to the primary vertex divided by its uncertainty, for the two lowest $p_{\mathrm{T}}$ leptons of the quadruplet in events with $m_{4 \ell}<190 \mathrm{GeV}$ is required to be less than 3.5 and 6 for muons and electrons respectively. The selection efficiency of the isolation and impact parameter requirements has been studied using data both for isolated leptons, with $Z \rightarrow \ell \ell$ decays and non-isolated leptons from semi-leptonic $b$ - and $c$-quark decays in a heavy-flavour enriched dijet sample. Good agreement is observed between data and simulation.

Higgs boson candidates are searched by selecting two sameflavour, opposite-sign isolated lepton pairs in an event. Each lepton must satisfy $p_{\mathrm{T}}>7 \mathrm{GeV}$ and be measured in the pseudorapidity range $|\eta|<2.47$ for electrons and $|\eta|<2.5$ for muons. The electron $p_{\mathrm{T}}$ threshold is increased to 15 GeV in the transition region between the barrel and end-cap calorimeters ( $1.37<|\eta|<1.52$ ). At least two leptons must have $p_{\mathrm{T}}>20 \mathrm{GeV}$. The leptons are required to be well separated from each other with $\Delta R>0.1$. The invariant mass of the lepton pair closest to the nominal $Z$ boson mass $\left(m_{Z}\right)$ is denoted by $m_{12}$ and it is required that $\left|m_{Z}-m_{12}\right|<$ 15 GeV . The invariant mass of the remaining lepton pair, $m_{34}$, is required to be lower than 115 GeV and greater than a threshold depending on the reconstructed four lepton mass, $m_{4 \ell}$, as summarized in Table 2. The final discriminating variable is $m_{4 \ell}$, where the Higgs boson production would appear as a clustering of events. The width of the reconstructed Higgs boson mass distribution is dominated by experimental resolution at low $m_{H}$ values,

Table 2
Thresholds applied to $m_{34}$ for reference values of $m_{4 \ell}$ (see text). For other $m_{4 \ell}$ values, the selection requirement is obtained via linear interpolation.

| $m_{4 \ell}(\mathrm{GeV})$ | $\leqslant 120$ | 130 | 140 | 150 | 160 | 165 | 180 | 190 | 200 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| Threshold $(\mathrm{GeV})$ | 15 | 20 | 25 | 30 | 30 | 35 | 40 | 50 | 60 |

Table 3
The expected numbers of background events, with their systematic uncertainty, separated into "Low mass" ( $m_{4 \ell}<180 \mathrm{GeV}$ ) and "High mass" ( $m_{4 \ell} \geqslant 180 \mathrm{GeV}$ ) regions. The expected numbers of signal events for different $m_{H}$ hypotheses and the observed numbers of events are also presented.

|  | $\mu \mu \mu \mu$ |  | ее $\mu \mu$ |  | ееее |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Low mass | High mass | Low mass | High mass | Low mass | High mass |
| Integrated luminosity | $2.28 \mathrm{fb}^{-1}$ |  | $1.96 \mathrm{fb}^{-1}$ |  | $1.98 \mathrm{fb}^{-1}$ |  |
| ZZ ${ }^{(*)}$ | $1.02 \pm 0.15$ | $7.7 \pm 1.2$ | $0.99 \pm 0.16$ | $9.6 \pm 1.4$ | $0.39 \pm 0.09$ | $3.6 \pm 0.5$ |
| $Z, Z b \bar{b}, t \bar{t}$ | $0.06 \pm 0.01$ | $0.01 \pm 0.01$ | $0.29 \pm 0.11$ | $0.15 \pm 0.06$ | $0.23 \pm 0.09$ | $0.12 \pm 0.05$ |
| Total background | $1.08 \pm 0.15$ | $7.7 \pm 1.2$ | $1.28 \pm 0.19$ | $9.8 \pm 1.4$ | $0.62 \pm 0.13$ | $3.7 \pm 0.5$ |
| Data | 1 | 11 | 1 | 8 | 1 | 5 |
| $m_{H}=130 \mathrm{GeV}$ | $0.42 \pm 0.07$ |  | $0.40 \pm 0.06$ |  | $0.14 \pm 0.03$ |  |
| $m_{H}=150 \mathrm{GeV}$ | $0.98 \pm 0.15$ |  | $0.97 \pm 0.15$ |  | $0.34 \pm 0.06$ |  |
| $m_{H}=200 \mathrm{GeV}$ |  | $2.26 \pm 0.33$ |  | $2.64 \pm 0.38$ |  | $0.98 \pm 0.14$ |
| $m_{H}=240 \mathrm{GeV}$ |  | $1.74 \pm 0.25$ |  | $2.24 \pm 0.32$ |  | $0.88 \pm 0.13$ |
| $m_{H}=300 \mathrm{GeV}$ |  | $1.18 \pm 0.17$ |  | $1.64 \pm 0.23$ |  | $0.64 \pm 0.09$ |
| $m_{H}=400 \mathrm{GeV}$ |  | $0.86 \pm 0.13$ |  | $1.23 \pm 0.18$ |  | $0.52 \pm 0.08$ |
| $m_{H}=600 \mathrm{GeV}$ |  | $0.15 \pm 0.02$ |  | $0.23 \pm 0.04$ |  | $0.10 \pm 0.02$ |

with a full-width at half-maximum (FWHM) which varies according to decay mode and is between $4.5(4 \mu)$ and 6.5 ( $4 e) \mathrm{GeV}$ for $m_{H}=130 \mathrm{GeV}$. At high $m_{H}$ the reconstructed width is dominated by the natural width of the Higgs boson with a FWHM of approximately 35 GeV at $m_{H}=400 \mathrm{GeV}$.

## 5. Background estimation

The dominant $Z Z^{(*)}$ background is estimated using MC simulation. Generated events are required to pass the complete analysis selection and the final yield is normalized to the integrated luminosity.

The $t \bar{t}$ background is also estimated using MC simulation. Comparison of data to MC predictions, in a control sample of events with opposite sign electron-muon pairs consistent with the $Z$ boson mass and with one or two additional charged leptons, are used to verify that the $t \bar{t}$ background is small with respect to the dominant $Z Z^{(*)}$ process and in agreement with expectation.

The $Z+$ jets background is normalized using data. The control sample is formed by selecting events with a pair of sameflavour, opposite-sign isolated leptons consistent with the $Z$ boson mass, $\left|m_{Z}-m_{12}\right|<15 \mathrm{GeV}$, and a second same-flavour, oppositesign lepton pair where only kinematic, but no isolation or impact parameter, requirements are applied. At this stage, the dominant background source depends on the flavour of the second lepton pair: $Z+$ light flavour jets dominates the final states with a second electron pair, while $Z b \bar{b}$ production dominates the final states with a second muon pair after the contributions from $t \bar{t}, Z Z^{(*)}$, and muons from in-flight $\pi$ and $K$ decays which correspond to $44 \%$ of the event yield are subtracted. The observed background, which is found to be in good agreement with expectation, is extrapolated to the signal region by means of the MC simulation.

## 6. Systematic uncertainties

Uncertainties on lepton reconstruction and identification efficiency, and on the momentum resolution and momentum scale
are determined using samples of $W, Z$ and $J / \psi$ decays. The muon efficiency uncertainty results in an acceptance uncertainty on the signal and the irreducible background which is uniform over the mass range of interest and amounts to $1.7 \%$ (1.2\%) for the $4 \mu$ $(2 e 2 \mu)$ channel. The uncertainty on the electron efficiency results in an acceptance uncertainty of $3 \%(2 \%)$ for the $4 e(2 e 2 \mu)$ channel at $m_{4 \ell}=600 \mathrm{GeV}$ reaching $15 \%(6 \%)$ at $m_{4 \ell}=110 \mathrm{GeV}$.

A conservative theoretical uncertainty of $15 \%$ is assigned to the $Z Z^{(*)}$ background contribution [44]. The $Z+$ light flavour jets and $Z b \bar{b}$ backgrounds are evaluated using data. A systematic uncertainty between $20 \%$ and $40 \%$ is assigned on their normalization to account for the statistical uncertainty in the control sample and the MC-based extrapolation to the signal region. The uncertainty on the $t \bar{t}$ cross section is found to be $10 \%$ by adding linearly the contributions from variations of the renormalization and factorization scales to those of the parton distribution functions.

The theoretical uncertainties on the Higgs boson production cross section are $15-20 \%$ for the gluon fusion process and $3-9 \%$ for the vector-boson fusion process [17], depending on the Higgs boson mass. ${ }^{2}$ They include uncertainties on the QCD scale and on the parton distribution functions [46-49]. An additional $2 \%$ uncertainty is added to the signal selection efficiency due to the modelling of the signal kinematics. This is evaluated by comparing signal samples generated with PYTHIA and the default powheg samples.

The overall uncertainty on the total integrated luminosity is 3.7\% [8].

## 7. Results

The number of events observed in each final state, separately for $m_{4 \ell}<180 \mathrm{GeV}$ and $m_{4 \ell} \geqslant 180 \mathrm{GeV}$, are compared with the ex-

[^14]

Fig. 1. Invariant mass distributions (a) $m_{12}$, (b) $m_{34}$, and (c) $m_{4 \ell}$ for the selected candidates. The data (dots) are compared to the background expectations from the dominant $Z Z^{(*)}$ process and the sum of $t \bar{t}, Z b \bar{b}$ and $Z+$ light flavour jets processes. Error bars represent $68.3 \%$ central confidence intervals.


Fig. 2. $m_{4 \ell}$ distribution of the selected candidates, compared to the background expectation. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for three $m_{H}$ hypotheses is also shown.
pectations for background and signal for various $m_{H}$ hypotheses in Table 3. In total 27 candidate events are selected by the analysis: $124 \mu, 92 e 2 \mu$, and $64 e$ events, while in the same mass range $24 \pm 4$ events are expected from the background processes. The $m_{12}, m_{34}$, and $m_{4 \ell}$ mass spectra are shown in Fig. 1. The $m_{4 \ell}$ distribution for the total background and several signal hypotheses is compared to the data in Fig. 2. The selected events have been examined visually and no evidence for reconstruction problems was identified.

Upper limits are set on the Higgs boson cross section at 95\% CL, using the $C L_{s}$ modified frequentist formalism [50] with the profile likelihood test statistic [51]. The test statistic is evaluated with a maximum likelihood fit of signal and background models to the observed $m_{4 \ell}$ distribution. Fig. 3 shows the expected and observed $95 \%$ CL cross section upper limits as a function of $m_{H}$ and Table 4 summarizes the numerical values for selected $m_{H}$ points. The consistency with the background-only hypothesis is quantified using the $p$-value, the probability that a background-only experiment fluctuates more than the observation. The most significant deviation from the background-only hypothesis is observed for $m_{H}=242 \mathrm{GeV}$ with a $p$-value of $4.9 \%$. These results do not account for the so-called "look-elsewhere" effect [52]. The SM Higgs


Fig. 3. The expected (dashed) and observed (full line) $95 \%$ CL upper limits on the Higgs boson production cross section as a function of the Higgs boson mass, divided by the expected SM Higgs boson cross section. The green and yellow bands indicate the expected sensitivity with $\pm 1 \sigma$ and $\pm 2 \sigma$ fluctuations, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this Letter.)

Table 4
Median expected and observed 95\% CL upper limits on the Higgs boson production cross section for several Higgs boson masses, divided by the expected SM Higgs boson cross section.

| Mass $(\mathrm{GeV})$ | Expected | Observed |
| :--- | :--- | :---: |
| 130 | 3.29 | 4.11 |
| 150 | 1.39 | 1.47 |
| 200 | 1.03 | 0.96 |
| 240 | 1.28 | 2.03 |
| 300 | 1.51 | 1.54 |
| 400 | 1.91 | 1.77 |
| 600 | 8.40 | 12.34 |

boson is excluded at $95 \%$ CL in the mass ranges 191-197, 199-200 and $214-224 \mathrm{GeV}$.

## 8. Summary

A search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ based on $2.1 \mathrm{fb}^{-1}$ of data recorded by the

ATLAS detector at $\sqrt{s}=7 \mathrm{TeV}$ during the 2011 run, has been presented. No significant excess of candidates is observed in the mass range between 110 and 600 GeV with respect to the expected SM background. The observed (expected) 95\% CL upper limit on the Higgs boson production cross section, in units of the SM cross section, is 0.99 (1.01) for $m_{H}=194 \mathrm{GeV}$, the region with the best expected sensitivity for this search. The SM Higgs boson is excluded at $95 \%$ CL in the mass ranges 191-197, 199-200 and $214-224 \mathrm{GeV}$.

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# Measurement of the inclusive isolated prompt photon cross-section in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ using $35 \mathrm{pb}^{-1}$ of ATLAS data ${ }^{\hat{4}}$ 

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#### Abstract

A measurement of the differential cross-section for the inclusive production of isolated prompt photons in $p p$ collisions at a center-of-mass energy $\sqrt{s}=7 \mathrm{TeV}$ is presented. The measurement covers the pseudorapidity ranges $|\eta|<1.37$ and $1.52 \leqslant|\eta|<2.37$ in the transverse energy range $45 \leqslant E_{\mathrm{T}}<$ 400 GeV . The results are based on an integrated luminosity of $35 \mathrm{pb}^{-1}$, collected with the ATLAS detector at the LHC. The yields of the signal photons are measured using a data-driven technique, based on the observed distribution of the hadronic energy in a narrow cone around the photon candidate and the photon selection criteria. The results are compared with next-to-leading order perturbative QCD calculations and found to be in good agreement over four orders of magnitude in cross-section.


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The production of prompt photons at hadron colliders provides means for testing perturbative QCD predictions [1], providing a colorless probe of the hard scattering process. The measurement of the inclusive production of prompt photons could be used to constrain the parton distribution functions; in particular it is sensitive to the gluon content of the proton [2] through the $q g \rightarrow q \gamma$ subprocess, which at leading order dominates the inclusive prompt photon cross-section at the LHC.

ATLAS has recently published a measurement of the inclusive photon cross-section in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ using an integrated luminosity of $880 \mathrm{nb}^{-1}$ [3]; a similar measurement has been performed by the CMS Collaboration [4] using an integrated luminosity of $2.9 \mathrm{pb}^{-1}$. Analogous measurements have been perfomed in $p \bar{p}$ collisions at a lower center of mass at the Tevatron [5,6], and in deep inelastic ep scattering at HERA [7,8]. This Letter presents the measurement of the differential production crosssection of isolated prompt photons with transverse energies $E_{\mathrm{T}}$ above 45 GeV using $34.6 \pm 1.2 \mathrm{pb}^{-1}$ of $p p$ collision data at $\sqrt{s}=$ 7 TeV collected in 2010. Isolated prompt photons in the pseudorapidity ranges $|\eta|<0.6,0.6 \leqslant|\eta|<1.37,1.52 \leqslant|\eta|<1.81$ and $1.81 \leqslant|\eta|<2.37$ are studied. ${ }^{1}$

[^15]In the following, all photons produced in $p p$ collisions and not coming from hadron decays are considered as prompt: they include both direct photons, which originate from the hard subprocess, and fragmentation photons, which are the result of the fragmentation of a colored high- $p_{\mathrm{T}}$ parton [9,10]. Isolated photons are considered: from a theoretical perspective, photons are isolated if the transverse energy $E_{\mathrm{T}}^{\text {iso }}$, within a cone of radius $R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}=0.4$ centered around the photon direction in the pseudorapidity $(\eta)$ and azimuthal angle $(\phi)$ plane, ${ }^{2}$ is smaller than $E_{\mathrm{T}}^{\text {cut }}$. In Jetphox [9], used for next-to-leading order (NLO) calculations, $E_{\mathrm{T}}^{\text {iso }}$ is calculated from all partons. Similarly, a corresponding isolation prescription is applied experimentally on the reconstructed objects, based on the energy reconstructed in an $R=0.4$ cone around the photon candidate, corrected for the effects associated with: the energy of the photon candidate itself, the underlying event and the collision pileup [3]. The main background to these isolated prompt photons is composed of photons from decays of light neutral mesons, such as the $\pi^{0}$ or $\eta$.

Photons are detected in ATLAS by a lead-liquid Argon sampling electromagnetic calorimeter (ECAL) with an accordion geometry, divided into a barrel section covering the pseudorapidity region $|\eta|<1.475$ and two endcap sections covering the pseudorapidity regions $1.375<|\eta|<3.2$. It consists of three longitudinal layers. The first layer has a high granularity along the $\eta$ direction (between 0.003 and 0.006 depending on $\eta$, with the exception of the regions $1.4<|\eta|<1.5$ and $|\eta|>2.4$ ), sufficient to provide an event-by-event discrimination between single photon showers and

[^16]showers coming from a $\pi^{0}$ decay. The second layer has a granularity of $0.025 \times 0.025$ in $\eta \times \phi$. A third layer is used to correct for the leakage beyond the electromagnetic calorimeter for highenergy showers, while in front of the accordion calorimeter a thin presampler layer, covering the pseudorapidity interval $|\eta|<1.8$, is used to correct for the energy absorbed before the calorimeter.

The ECAL energy resolution is parametrized as $\sigma(E) / E=$ $a / \sqrt{E(\mathrm{GeV})} \oplus c$ with the largest contribution coming from the sampling term $a$, corresponding to approximately $10 \%$ (20\%) in the barrel (endcap) region. For energies above 200 GeV the global constant term $c$, estimated to be $(1.2 \pm 0.6) \%((1.8 \pm 0.6) \%)$ in the barrel (endcap) for the 2010 data, starts to dominate [11]. In front of the electromagnetic calorimeter the inner detector allows the reconstruction of tracks from the primary $p p$ collision point and also from secondary vertices, permitting an efficient reconstruction of photon conversions in the beam pipe and inner detector up to a radius of $\sim 80 \mathrm{~cm}$. Further details of the inner detector, the electromagnetic calorimeter and the whole ATLAS detector are documented in Ref. [12].

Event samples simulated with Pythia 6.4.21 [13] are used to study the characteristics of signal and background events. To estimate systematic uncertainties related to the choice of the event generator and the parton shower model, alternative samples are generated with Herwig 6.5 [14]. Events used in this analysis are triggered using a single-photon trigger with a nominal transverse energy threshold of 40 GeV . The trigger efficiency, $\varepsilon^{\text {trig }}$, is measured using a bootstrap method to be $\left(99.4_{-0.2}^{+0.6}\right) \%$ for prompt photon candidates with $E_{\mathrm{T}}>45 \mathrm{GeV}$ passing the selection criteria presented below. The same trigger condition was used for the whole dataset, even though the mean number of events per collision rose from $<1$ to $\sim 3$ as the instantaneous luminosity increased during 2010. Collision candidates are selected by requiring a primary vertex with at least three associated charged particle tracks, consistent with the beam interaction region. The total number of selected events in data after these requirements is almost 1.7 million, with a negligible amount of non-collision background.

Photon candidates are formed from clusters of energy deposits reconstructed in the electromagnetic calorimeter [15]. Clusters without matching tracks are classified as unconverted photon candidates. The presence of one or two tracks coming from a conversion vertex is used to distinguish converted photons from electrons. Converted photon clusters are rebuilt with a wider size in $\phi$, to account for the opening angle between the conversion products due to the magnetic field. A specific energy calibration [15] is then applied separately for converted and unconverted photon candidates to account for energy loss in front of the ECAL and both lateral and longitudinal leakage. Photon clusters are removed if their barycenter lies in the transition between the barrel and endcap regions of the electromagnetic calorimeter, corresponding to $1.37<|\eta|<$ 1.52, where larger uncertainties related to the efficiency measurement are expected. Clusters containing cells overlapping with the small number of regions with problematic calorimeter readout or with very noisy cells are also removed. Over 0.8 million photon candidates with $E_{\mathrm{T}}>45 \mathrm{GeV}$ remain in the data sample.

A measurement of the transverse isolation energy $E_{\mathrm{T}}^{\text {iso }}$ is associated with each photon candidate, computed by summing the calorimeter energy in a cone of $R=0.4$ around the candidate, as detailed in Ref. [3]. Corrections to this isolation energy are derived from simulation to remove the energy of the photon itself that leaks into the isolation cone. An event-by-event correction [16,17] is applied to subtract the estimated contributions from the underlying event and in-time pileup (i.e. from additional proton-proton interactions). The correction to $E_{\mathrm{T}}^{\mathrm{iso}}$ is typically 900 MeV . After this subtraction, the remaining fluctuations are dominated by electronic noise from the calorimeter measurement. The effect of the out-
of-time pileup, associated with collisions taking place in previous bunch-crossings, is found to be minimal (i.e. shifts of 200 MeV at most, towards lower isolation energies). The corrections mentioned above allow $E_{\mathrm{T}}^{\text {iso }}$ to be directly compared to parton-level theoretical predictions.

All photon candidates having reconstructed isolation energy $<3 \mathrm{GeV}$ are considered as experimentally isolated. This definition is similar to applying a 4 GeV cut on the particle-level isolation, defined as the transverse energy of all stable particles in a cone of radius $R=0.4$ around the photon direction (with the underlying event removed as before). The small difference between the two, caused by noise and other detector effects, is taken into account in the uncertainties associated with the photon reconstruction efficiency $\varepsilon^{\text {reco }}$ discussed below. The particle-level isolation can in turn be related to the parton-level isolation in Jetphox that is used for the NLO predictions. The efficiency of the isolation criteria is found to be similar (i.e. within a few percent) at both the particle-level and the parton-level for simulated photons passing the selection described below.

As in Ref. [3], the reconstruction and preselection efficiency $\varepsilon^{\text {reco }}$ is computed from simulated prompt photons as a function of the true photon $E_{\mathrm{T}}$. It is defined as the ratio between the number of photons reconstructed in a given $|\eta|$ interval with reconstructed $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$, and the total number of true prompt photons with true pseudorapidity in the same $|\eta|$ interval, and with particlelevel transverse isolation energy $<4 \mathrm{GeV}$. The estimated $\varepsilon^{\text {reco }}$ for photons with $45<E_{\mathrm{T}}<400 \mathrm{GeV}$ is $\sim 85 \%$ (75\%) in the barrel (endcap) region. The main inefficiency $(\sim 10 \%)$ is due to the acceptance loss originating from a few inoperative optical links in the calorimeter readout. A similar reduction is caused by the isolation requirement in the pseudorapidity region $1.52 \leqslant|\eta|<1.81$ where the calorimetric isolation suffers from larger detector effects. The systematic uncertainty on $\varepsilon^{\text {reco }}$ associated with the experimental isolation requirement is evaluated from the prompt photon simulation by varying the value of the isolation criterion by the average difference $(\sim 500 \mathrm{MeV})$ observed for electrons from $W \rightarrow e v$ events in data and simulation. The estimated uncertainty varies between 3 and $4 \%$ depending on $\eta$. The uncertainty associated with the imperfect knowledge of the material in front of the ECAL is estimated by comparing the expected efficiencies in a sample simulated with the nominal ATLAS setup, and one with increased material. It varies between 1 and $2.5 \%$, depending on $\eta$.

Shape variables computed from the lateral and longitudinal energy profiles of the shower in the calorimeters are used to discriminate signal from background [15,18]. As detailed in Ref. [3], selection criteria on these variables, optimized independently for unconverted and converted photons, are applied to reconstructed photon candidates. The requirements on these variables are applied in stages resulting in tight candidates: firstly jets are removed whilst still keeping a high photon efficiency and then secondly wide or closely spaced showers (i.e. those consistent with jets or meson decays) are rejected. The selection criteria have been revised to minimize the systematics on the efficiency extraction, especially in the region $1.81 \leqslant|\eta|<2.37$. The photon identification efficiency $\varepsilon^{\mathrm{ID}}$ is computed from simulation as a function of transverse energy in each pseudorapidity region. It is defined as the efficiency for reconstructed (true) prompt photons, with measured $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$, to pass the identification criteria mentioned above.

Following the same method as in Ref. [3], the value of $\varepsilon^{\mathrm{ID}}$ is determined after correcting the simulated shower shapes for the observed average differences with respect to data. In the present analysis, however, the corrections are estimated for unconverted and converted photons separately. This helps to reduce the systematic uncertainties associated with the correction procedure. The


Fig. 1. Distributions of $E_{\mathrm{T}}^{\text {iso }}$ for photon candidates with $45<E_{\mathrm{T}}<55 \mathrm{GeV}$ in $|\eta|<$ 0.6 passing the tight (solid dots) and non-tight (open triangles) shower-shape-based selection criteria. The non-tight distribution is normalized to the tight distribution for $E_{\mathrm{T}}^{\text {iso }}>5 \mathrm{GeV}$ (non-isolated region), where the signal contamination is fairly small.
value of $\varepsilon^{\mathrm{ID}}$ varies from 90 to $97 \%$, depending on $\eta$ and increasing with $E_{\mathrm{T}}$. The systematic uncertainty on $\varepsilon^{\mathrm{ID}}$ is also $\eta$ dependent, ranging from 1.5 to $3 \%$, with contributions from: detector simulation; background contamination; (un)converted photon misclassification; direct/fragmentation photon fraction; the choice of different Monte Carlo generators (MC). These uncertainties affect the reconstruction and identification efficiencies in a correlated way, and are treated as such in their combination. After applying the isolation criterion and the tight selection on the shape variables, almost 173,000 photon candidates remain in the data sample.

As in Ref. [3], a two-dimensional-sideband method is used to estimate the background contribution from data and to measure the prompt photon signal yield. The two dimensions are the transverse isolation energy $E_{\mathrm{T}}^{\text {iso }}$ and the quality of the photon, defined by whether or not it passes the shower shape identification criteria. On the isolation axis, the signal region contains photon candidates with $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$, while the sideband region contains nonisolated photon candidates with $E_{\mathrm{T}}^{\text {iso }}>5 \mathrm{GeV}$. On the other axis, the signal photon candidates are required to pass the tight identification criteria (tight candidates). Those failing the tight criteria but passing a background-enriching subset of these criteria (non-tight candidates) are contained in the sideband. A typical distribution of $E_{\mathrm{T}}^{\text {iso }}$ for both tight and non-tight data is shown in Fig. 1 for photon candidates with $45<E_{\mathrm{T}}<55 \mathrm{GeV}$ in $|\eta|<0.6$. The non-tight distribution is normalized to the tight one above 5 GeV where a only small signal contamination is expected.

Corrections for the signal contamination in the background control regions are computed using prompt photon Monte Carlo samples. For the tight isolated signal leaking into the non-isolated region, these are as large as $17 \%$ at high $E_{\mathrm{T}}$. Smaller leakages of up to $6 \%$ are expected for the other two background control regions. The purity of isolated prompt photons measured with this method increases with $E_{\mathrm{T}}$ from $91 \%$ at $E_{\mathrm{T}}=45 \mathrm{GeV}$ to close to $100 \%$ at $E_{\mathrm{T}}>200 \mathrm{GeV}$.

The main contributions to the uncertainty on the yields come from the fragmentation fraction ( $\lesssim 8 \%$ ), estimated by conservatively varying the fraction from 0 to $100 \%$ in the signal sample, and pileup ( $5 \%$, with fluctuations up to $8 \%$ for $1.52 \leqslant|\eta|<1.81$ ), estimated by increasing the correction to $E_{\mathrm{T}}^{\text {iso }}$ by $50 \%$ both in data and simulation. This scaling of the correction minimizes the residual dependency of the isolation on the number of primary vertices
(i.e. pileup) in data. The other contributions to the uncertainty are: correlated background in the two-dimensional-sideband regions ( $\lesssim 5 \%$ barrel and $\lesssim 10 \%$ endcap, $E_{\mathrm{T}}$ dependent), definition of the two-dimensional-sideband regions ( $\lesssim 5 \%$ non-tight and $1 \%$ non-isolated), photon energy scale ( $2-8 \%, \eta$ dependent), slightly narrower showers in simulation than in data $\left(2-5 \%, \eta\right.$ and $E_{\mathrm{T}}$ dependent), isolation shower leakage corrections (1-5\%), Monte Carlo generator ( $2 \%$ ), material effects ( $<1 \%$ ), and prompt electron misidentification ( $\sim 0.5 \%$, varying with $E_{\mathrm{T}}$ ). Globally, the uncertainties on the photon signal yields are less than $10 \%$, and decrease with $E_{\mathrm{T}}$.

The average differential cross-section $\left\langle d \sigma_{j}^{k} / d E_{\mathrm{T}}^{\text {true }}\right\rangle$ for the production of isolated prompt photons in a bin $j$ of $E_{\mathrm{T}}^{\text {true }}$ (integrated over one true $|\eta|$ bin $k$ ) is related to the signal yield $N_{i}^{\gamma, \text { reco, } k}$ (in the $k$ th $|\eta|$ bin and $i$ th $E_{\mathrm{T}}$ bin) by the relationship:

$$
\begin{align*}
N_{i}^{\gamma, \text { reco }, k}= & \left(\int \mathcal{L} d t\right) \varepsilon^{\mathrm{trig}} \varepsilon_{i}^{\mathrm{ID}, k} \\
& \times \sum_{j} R_{i j}^{k} \varepsilon_{j}^{\mathrm{reco}, k} \Delta E_{\mathrm{T}, j}^{\mathrm{true}}\left\langle\frac{d \sigma_{j}^{k}}{d E_{\mathrm{T}}^{\mathrm{true}}}\right\rangle \tag{1}
\end{align*}
$$

where $\varepsilon_{i}^{\mathrm{ID}, k}$ is the average identification efficiency and $R_{i j}^{k}$ is the $E_{\mathrm{T}}$ response matrix. The elements of $R_{i j}^{k}$ are evaluated from the ratio of the true to reconstructed $E_{\mathrm{T}}$ distributions of photon candidates, using simulated samples of isolated prompt photons. The migration from one $E_{\mathrm{T}}$ bin to another is less than $10 \%$ in most $E_{\mathrm{T}}$ and $\eta$ regions. A larger migration of up to $18 \%$ is observed in the region $1.52 \leqslant|\eta|<1.81$, where more material is present in front of the electromagnetic calorimeter. Migrations between $\eta$ bins are neglected given the large bin size and the excellent ECAL $\eta$ resolution. A singular value decomposition (SVD) [19] is used to unfold the $E_{\mathrm{T}}$ distribution for detector effects. The regularization of the resulting unfolded distribution is tuned using simulated events and chosen to be very loose to avoid a potential bias toward the truth reference spectrum. The simulation model dependence is tested with pseudo-experiments, using Pythia and Herwig simulated samples. The difference of the unfolded crosssection obtained in both cases is found to be $<3 \%$. The uncertainty associated with the ECAL energy resolution is $\sim 1 \%$. The lower and upper $E_{\mathrm{T}}$ constraints have negligible effect on the unfolded spectrum.

The measured inclusive isolated prompt photon production cross-sections are shown in Fig. 2. They are presented as a function of the photon transverse energy, for each of the four considered pseudorapidity intervals. They are also presented in tabular form in Appendix A. The error bars on the data points represent the combination of the statistical and systematic uncertainties: systematic uncertainties dominate over the entire kinematic range considered. The contribution from the luminosity uncertainty (3.4\%) is shown separately as it represents a possible global change by a common multiplicative factor. The data agree with NLO pQCD calculations, obtained with JeTphox 1.2.2 [9] using the CTEQ 6.6 PDFs [20] and the BFG set II [21] fragmentation functions (FF). These predictions are negligibly affected when using BFG set I instead. The nominal renormalization, factorization and fragmentation scales are set to the $E_{\mathrm{T}}$ of the photon. Theoretical calculations using MSTW 2008 [22] and NNPDF2.0 [23] PDFs show a similarly good agreement to data. The central values obtained with the MSTW 2008 (NNPDF2.0) PDFs are 3 to 5\% ( 1 to $4 \%$ ) higher than those predicted using the CTEQ 6.6 PDFs. The total systematic uncertainties on the theoretical predictions are represented with a solid band. The scale uncertainty ( $\sim 10 \%$ ) is the leading theoretical systematic uncertainty. It is estimated from the enve-


Fig. 2. Measured (dots) and expected (shaded area) inclusive prompt photon production cross-sections, and their ratio, as a function of the photon $E_{T}$ and in the range (a) $|\eta|<0.6$, (b) $0.6 \leqslant|\eta|<1.37$, (c) $1.52 \leqslant|\eta|<1.81$ and (d) $1.81 \leqslant|\eta|<2.37$. The data error bars combine the statistical and systematic uncertainties, with the luminosity uncertainty shown separately (dotted bands).
lope of independent and coherent variations of the three scales, by a factor of two around the central value, with the renormalization scale (coherent variation) dominating this envelope at low (high) $E_{\mathrm{T}}$, while the fragmentation scale produces the smallest variation. The scale error is summed in quadrature with the contributions from the PDF uncertainty ( $5 \%$ at $68 \%$ C.L.) and the uncertainty associated with the choice of the parton-level isolation criterion (2\%). The same quantities are also shown in the bottom panels after having been normalized to the expected NLO pQCD cross-sections.

In conclusion, the inclusive isolated prompt photon production cross-section in $p p$ collisions at a center-of-mass energy $\sqrt{s}=$ 7 TeV has been measured using $35 \mathrm{pb}^{-1}$ of integrated luminosity collected by the ATLAS detector at the LHC. The differential crosssection has been measured as a function of the prompt photon transverse energy between 45 and 400 GeV , in the pseudorapidity ranges $0.0 \leqslant|\eta|<0.6,0.6 \leqslant|\eta|<1.37,1.52 \leqslant|\eta|<1.81$ and $1.81 \leqslant|\eta|<2.37$. In general, good agreement between the data and the NLO pQCD predictions is observed. This measurement improves the precision and significantly extends the kinematic
regime explored in the previous measurement [3] and is consistent in the region where the two measurements overlap.

Over most of this extended kinematic range the experimental errors are smaller than the theoretical ones. The large theoretical scale error limits the discrimination between PDFs. Future measurements of this process in finer pseudorapidity binning and those of the photon + jet system should provide more insight into the PDF differences.

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Table A. 1
 uncertainties (summed in quadrature), except for the uncertainty on the luminosity.

| $\begin{aligned} & E_{\mathrm{T}}^{\min } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & E_{\mathrm{T}}^{\max } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & d \sigma / d E_{\mathrm{T}} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {stat }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\delta_{\text {yield }}$ [pb/GeV] | $\delta_{\text {efficiency }}$ [pb/GeV] | $\begin{aligned} & \delta_{\text {corr }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {unfolding }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {tot }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {lumi }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 45 | 55 | 83.3 | 0.5 | 4.8 | 3.3 | 3.4 | 2.5 | 7.2 | 2.8 |
| 55 | 70 | 32.7 | 0.3 | 1.8 | 1.2 | 1.2 | 1.0 | 2.7 | 1.1 |
| 70 | 85 | 12.3 | 0.2 | 0.6 | 0.4 | 0.4 | 0.4 | 0.9 | 0.4 |
| 85 | 100 | 5.3 | 0.1 | 0.2 | 0.2 | 0.2 | 0.2 | 0.4 | 0.2 |
| 100 | 125 | 2.2 | 0.05 | 0.09 | 0.08 | 0.07 | 0.07 | 0.2 | 0.07 |
| 125 | 150 | 0.80 | 0.03 | 0.03 | 0.03 | 0.02 | 0.03 | 0.06 | 0.03 |
| 150 | 200 | 0.26 | 0.01 | 0.01 | $9 \times 10^{-3}$ | $7 \times 10^{-3}$ | $8 \times 10^{-3}$ | 0.02 | $9 \times 10^{-3}$ |
| 200 | 400 | $2.8 \times 10^{-2}$ | $2 \times 10^{-3}$ | $2 \times 10^{-3}$ | $1 \times 10^{-3}$ | $4 \times 10^{-4}$ | $8 \times 10^{-4}$ | $3 \times 10^{-3}$ | $9 \times 10^{-4}$ |

Table A. 2
Measured isolated prompt photon cross-section for $0.6 \leqslant|\eta|<1.37$, uncertainties as in Table A.1.

| $\begin{aligned} & E_{\mathrm{T}}^{\min } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & E_{\mathrm{T}}^{\max } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & d \sigma / d E_{\mathrm{T}} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {stat }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {yield }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {efficiency }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {corr }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\delta_{\text {unfolding }}$ [pb/GeV] | $\begin{aligned} & \delta_{\text {tot }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {lumi }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 45 | 55 | 99.0 | 0.7 | 8.1 | 4.4 | 3.8 | 3.0 | 10.4 | 3.4 |
| 55 | 70 | 38.9 | 0.3 | 3.0 | 1.7 | 1.2 | 1.2 | 3.9 | 1.3 |
| 70 | 85 | 14.9 | 0.2 | 1.1 | 0.7 | 0.4 | 0.5 | 1.4 | 0.5 |
| 85 | 100 | 6.3 | 0.1 | 0.4 | 0.3 | 0.1 | 0.2 | 0.6 | 0.2 |
| 100 | 125 | 2.7 | 0.06 | 0.2 | 0.1 | 0.06 | 0.08 | 0.2 | 0.09 |
| 125 | 150 | 1.0 | 0.03 | 0.06 | 0.04 | 0.02 | 0.03 | 0.1 | 0.03 |
| 150 | 200 | 0.29 | 0.01 | 0.02 | 0.01 | $7 \times 10^{-3}$ | $9 \times 10^{-3}$ | 0.03 | 0.01 |
| 200 | 400 | $3.2 \times 10^{-2}$ | $2 \times 10^{-3}$ | $3 \times 10^{-3}$ | $2 \times 10^{-3}$ | $9 \times 10^{-4}$ | $1 \times 10^{-3}$ | $4 \times 10^{-3}$ | $1 \times 10^{-3}$ |

Table A. 3
Measured isolated prompt photon cross-section for $1.52 \leqslant|\eta|<1.81$, uncertainties as in Table A.1.

| $\begin{aligned} & E_{\mathrm{T}}^{\min } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & E_{\mathrm{T}}^{\max } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & d \sigma / d E_{\mathrm{T}} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {stat }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {yield }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\delta_{\text {efficiency }}$ <br> [pb/GeV] | $\begin{aligned} & \delta_{\text {corr }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\delta_{\text {unfolding }}$ [pb/GeV] | $\begin{aligned} & \delta_{\text {tot }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {lumi }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 45 | 55 | 41.9 | 0.4 | 4.6 | 3.1 | 1.2 | 1.3 | 5.8 | 1.4 |
| 55 | 70 | 15.7 | 0.2 | 1.6 | 1.0 | 0.4 | 0.5 | 2 | 0.5 |
| 70 | 85 | 6.4 | 0.2 | 0.5 | 0.4 | 0.2 | 0.2 | 0.7 | 0.2 |
| 85 | 100 | 2.4 | 0.08 | 0.2 | 0.2 | 0.05 | 0.08 | 0.3 | 0.08 |
| 100 | 125 | 1.0 | 0.04 | 0.07 | 0.08 | 0.02 | 0.03 | 0.1 | 0.03 |
| 125 | 150 | 0.36 | 0.02 | 0.03 | 0.03 | $8 \times 10^{-3}$ | 0.01 | 0.05 | 0.01 |
| 150 | 200 | 0.11 | $9 \times 10^{-3}$ | 0.01 | $7 \times 10^{-3}$ | $3 \times 10^{-3}$ | $4 \times 10^{-3}$ | 0.02 | $4 \times 10^{-3}$ |
| 200 | 400 | $1.1 \times 10^{-2}$ | $1 \times 10^{-3}$ | $1 \times 10^{-3}$ | $8 \times 10^{-4}$ | $2 \times 10^{-4}$ | $3 \times 10^{-4}$ | $2 \times 10^{-3}$ | $4 \times 10^{-4}$ |

Table A. 4
Measured isolated prompt photon cross-section for $1.81 \leqslant|\eta|<2.37$, uncertainties as in Table A.1.

| $\begin{aligned} & E_{\mathrm{T}}^{\min } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & E_{\mathrm{T}}^{\max } \\ & {[\mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & d \sigma / d E_{\mathrm{T}} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {stat }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\delta_{\text {yield }}$ [pb/GeV] | $\delta_{\text {efficiency }}$ [pb/GeV] | $\begin{aligned} & \delta_{\text {corr }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\delta_{\text {unfolding }}$ [pb/GeV] | $\begin{aligned} & \delta_{\text {tot }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ | $\begin{aligned} & \delta_{\text {lumi }} \\ & {[\mathrm{pb} / \mathrm{GeV}]} \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 45 | 55 | 68.9 | 0.6 | 7.6 | 3.8 | 3.9 | 2.1 | 9.6 | 2.3 |
| 55 | 70 | 26.4 | 0.3 | 2.7 | 1.3 | 1.3 | 0.8 | 3.3 | 0.9 |
| 70 | 85 | 10.0 | 0.2 | 0.9 | 0.5 | 0.5 | 0.3 | 1.2 | 0.3 |
| 85 | 100 | 4.2 | 0.1 | 0.3 | 0.3 | 0.2 | 0.1 | 0.5 | 0.1 |
| 100 | 125 | 1.7 | 0.06 | 0.1 | 0.1 | 0.08 | 0.05 | 0.2 | 0.06 |
| 125 | 150 | 0.55 | 0.03 | 0.03 | 0.03 | 0.02 | 0.02 | 0.06 | 0.02 |
| 150 | 200 | 0.17 | 0.01 | 0.01 | 0.01 | $6 \times 10^{-3}$ | $6 \times 10^{-3}$ | 0.02 | $6 \times 10^{-3}$ |
| 200 | 400 | $1.2 \times 10^{-2}$ | $1 \times 10^{-3}$ | $6 \times 10^{-4}$ | $3 \times 10^{-3}$ | $3 \times 10^{-4}$ | $4 \times 10^{-4}$ | $3 \times 10^{-3}$ | $4 \times 10^{-4}$ |

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## Appendix A. Cross-section measurements

Tables A.1-A. 4 list the values of the measured isolated prompt photon production cross-sections, for the $0.0 \leqslant|\eta|<0.6,0.6 \leqslant$ $|\eta|<1.37,1.52 \leqslant|\eta|<1.81$ and $1.81 \leqslant|\eta|<2.37$ regions, respectively. The various systematic uncertainties originating from the purity measurement, the photon selection and identification efficiency and the luminosity are shown. In addition, the correlated uncertainties between the efficiency and the purity determination
are propagated as such and included separately ( $\sigma_{\text {corr }}$ ). The total uncertainty is the combination of the statistical and systematic uncertainties (summed in quadrature), except for the uncertainty on the luminosity.

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# Search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ with $4.8 \mathrm{fb}^{-1}$ of $p p$ collision data at $\sqrt{s}=7 \mathrm{TeV}$ with ATLAS ${ }^{\pi}$ 

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#### Abstract

This Letter presents a search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow$ $\ell^{+} \ell^{-} \ell^{\prime+} \ell^{\prime-}$, where $\ell, \ell^{\prime}=e$ or $\mu$, using proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ recorded with the ATLAS detector and corresponding to an integrated luminosity of $4.8 \mathrm{fb}^{-1}$. The four-lepton invariant mass distribution is compared with Standard Model background expectations to derive upper limits on the cross section of a Standard Model Higgs boson with a mass between 110 GeV and 600 GeV . The mass ranges $134-156 \mathrm{GeV}, 182-233 \mathrm{GeV}, 256-265 \mathrm{GeV}$ and $268-415 \mathrm{GeV}$ are excluded at the $95 \%$ confidence level. The largest upward deviations from the background-only hypothesis are observed for Higgs boson masses of $125 \mathrm{GeV}, 244 \mathrm{GeV}$ and 500 GeV with local significances of 2.1, 2.2 and 2.1 standard deviations, respectively. Once the look-elsewhere effect is considered, none of these excesses are significant.


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## 1. Introduction

The search for the Standard Model (SM) Higgs boson [1-3] is one of the most important aspects of the CERN Large Hadron Collider (LHC) physics program. Direct searches performed at the CERN Large Electron-Positron Collider (LEP) excluded at 95\% confidence level (CL) the production of a SM Higgs boson with mass, $m_{H}$, less than 114.4 GeV [4]. The searches at the Fermilab Tevatron $p \bar{p}$ collider have excluded at $95 \%$ CL the region $156<$ $m_{H}<177 \mathrm{GeV}$ [5]. At the LHC, results from data collected in 2010 extended the search in the region $200<m_{H}<600 \mathrm{GeV}$ by excluding a Higgs boson with cross section larger than 5-20 times the SM prediction [6,7]. In ATLAS these results were extended further using the first $1.04-2.28 \mathrm{fb}^{-1}$ of data recorded in 2011 [8-13]. In particular, the $H \rightarrow W W^{(*)} \rightarrow \ell^{+} \nu \ell^{-} \bar{v}$ search [13] excluded at $95 \%$ CL the region $145<m_{H}<206 \mathrm{GeV}$.

The search for the SM Higgs boson through the decay $H \rightarrow$ $Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{\prime+} \ell^{\prime-}$, where $\ell, \ell^{\prime}=e$ or $\mu$, provides good sensitivity over a wide mass range. Previous results from ATLAS in this channel [9] excluded three mass regions between 191 GeV and 224 GeV at $95 \% \mathrm{CL}$ with a $2.1 \mathrm{fb}^{-1}$ data sample. This Letter presents an update of this search in the mass range from 110 GeV to 600 GeV , superseding Ref. [9]. Three distinct final states, $\mu^{+} \mu^{-} \mu^{+} \mu^{-}(4 \mu), e^{+} e^{-} \mu^{+} \mu^{-}(2 e 2 \mu)$, and $e^{+} e^{-} e^{+} e^{-}$(4e), are selected. The largest background to this search comes from continuum $\left(Z^{(*)} / \gamma^{*}\right)\left(Z^{(*)} / \gamma^{*}\right)$ production, referred to as $Z Z^{(*)}$ hereafter.

[^17]For $m_{H}<180 \mathrm{GeV}$, there are also important background contributions from $Z+$ jets and $t \bar{t}$ production, where the additional charged lepton candidates arise either from decays of hadrons with $b$ - or $c$-quark content or from misidentification of jets.

The $\sqrt{s}=7 \mathrm{TeV} p p$ collision data were recorded during 2011 with the ATLAS detector at the LHC and correspond to an integrated luminosity of $4.8 \mathrm{fb}^{-1}$ [14,15]. This analysis is using more than twice the integrated luminosity of Ref. [9], including the data therein. The electron identification efficiency has been improved; furthermore the electron tracks have been refitted using a Gaussian-sum filter [16], which corrects for energy losses due to bremsstrahlung. The analysis also benefits from recent significant improvements in the alignment of the inner detector and the muon spectrometer.

## 2. The ATLAS detector

The ATLAS detector [17] is a multi-purpose particle physics detector with forward-backward symmetric cylindrical geometry. ${ }^{1}$ The inner tracking detector (ID) [18] covers $|\eta|<2.5$ and consists of a silicon pixel detector, a silicon microstrip detector, and a transition radiation tracker. The ID is surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field. A high-granularity lead/liquid-argon (LAr) sampling

[^18]Table 1

 $m_{H}>300 \mathrm{GeV}$. The decay branching ratio for $H \rightarrow 4 \ell$, with $\ell=e$ or $\mu$, is reported in the last column [34].

| $m_{H}[\mathrm{GeV}]$ | $\sigma(g g \rightarrow H)[\mathrm{pb}]$ | $\sigma\left(q q^{\prime} \rightarrow H q q^{\prime}\right)[\mathrm{pb}]$ | $\sigma(q \bar{q} \rightarrow W H)[\mathrm{pb}]$ | $\sigma(q \bar{q} \rightarrow Z H)[\mathrm{pb}]$ | $\mathrm{BR}\left(H \rightarrow Z Z^{(*)} \rightarrow 4 \ell\right)\left[10^{-3}\right]$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 130 | $14.1_{-2.1}^{+2.7}$ | $1.154_{-0.027}^{+0.032}$ | $0.501 \pm 0.020$ | $0.278 \pm 0.014$ | 0.19 |
| 150 | $10.5{ }_{-1.6}^{+2.0}$ | $0.962_{-0.021}^{+0.028}$ | $0.300 \pm 0.012$ | $0.171 \pm 0.009$ | 0.38 |
| 200 | $5.2{ }_{-0.8}^{+0.9}$ | $0.637_{-0.015}^{+0.022}$ | $0.103 \pm 0.005$ | $0.061 \pm 0.004$ | 1.15 |
| 400 | $2.0 \pm 0.3$ | $0.162_{-0.005}^{+0.010}$ | - | - | 1.21 |
| 600 | $0.33 \pm 0.06$ | $0.058_{-0.002}^{+0.005}$ | - | - | 1.23 |

calorimeter [19] measures the energy and the position of electromagnetic showers with $|\eta|<3.2$. LAr sampling calorimeters are also used to measure hadronic showers in the end-cap ( $1.5<|\eta|<3.2$ ) and forward ( $3.1<|\eta|<4.9$ ) regions, while an iron/scintillator tile calorimeter [20] measures hadronic showers in the central region ( $|\eta|<1.7$ ). The muon spectrometer (MS) [21] surrounds the calorimeters and consists of three large superconducting air-core toroids, each with eight coils, a system of precision tracking chambers ( $|\eta|<2.7$ ), and fast tracking chambers for triggering. A three-level trigger system [22] selects events to be recorded for offline analysis.

## 3. Data and simulation samples

The data are subjected to quality requirements: events recorded during periods when the relevant detector components were not operating normally are rejected. The resulting integrated luminosity is $4.8 \mathrm{fb}^{-1}, 4.8 \mathrm{fb}^{-1}$ and $4.9 \mathrm{fb}^{-1}$ for the $4 \mu, 2 e 2 \mu$ and $4 e$ final states, respectively.

The $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ signal is modelled using the powheg Monte Carlo (MC) event generator [23,24], which calculates separately the gluon-gluon and vector-boson fusion production mechanisms with matrix elements up to next-to-leading order (NLO). The Higgs boson transverse momentum $\left(p_{\mathrm{T}}\right)$ spectrum in the gluon fusion process is reweighted to match the calculation of Ref. [25], which includes quantum chromodynamics (QCD) corrections up to NLO and QCD soft-gluon resummations up to next-to-next-toleading logarithm (NNLL). pOWHEG is interfaced to PYTHIA [26] for showering and hadronization, which in turn is interfaced to рнотоs [27] for quantum electrodynamics (QED) radiative corrections in the final state and to tauola $[28,29]$ for the simulation of $\tau$ lepton decays. pythia is used to simulate the production of a Higgs boson in association with a $W$ or a $Z$ boson.

The Higgs boson production cross sections and decay branching ratios [30-33], as well as their uncertainties, are taken from Refs. [34,35]. The cross sections for the gluon fusion process have been calculated at next-to-leading order (NLO) in QCD [36-38], and then at next-to-next-to-leading order (NNLO) [39-41]. In addition, QCD soft-gluon resummations up to NNLL are applied for the gluon fusion process [42]. The NLO electroweak (EW) corrections are applied $[43,44]$. These results are compiled in Refs. [45-47] assuming factorization between QCD and EW corrections. The cross sections for the vector-boson fusion process are calculated with full NLO QCD and EW corrections [48-50], and approximate NNLO QCD corrections are available [51]. The associated productions with a $W$ or $Z$ boson are calculated at NLO [52] and at NNLO [53] in QCD, and NLO EW radiative corrections [54] are applied. The uncertainty in the production cross section due to the choice of QCD scale is ${ }_{-8}^{+12} \%$ for the gluon fusion process, and $\pm 1 \%$ for the vector-boson fusion, associated WH production, and associated ZH production processes [34]. The uncertainty in the production cross section due to the parton distribution function (PDF) and $\alpha_{s}$ is $\pm 8 \%$ for gluoninitiated process and $\pm 4 \%$ for quark-initiated processes [55-59].

The Higgs boson decay branching ratio to the four-lepton final state is predicted by prophecy 4 F [31,32], which includes the complete NLO QCD + EW corrections, interference effects between identical final-state fermions, and leading two-loop heavy Higgs boson corrections to the four-fermion width. Table 1 gives the production cross sections and branching ratios for $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ for several Higgs boson masses.

The cross section calculations do not take into account the width of the Higgs boson, which is implemented through a relativistic Breit-Wigner line shape applied at the event-generator level. It has been suggested [35,60-62] that effects related to off-shell Higgs boson production and interference with other SM processes may become sizeable for the highest masses ( $m_{H}>$ 400 GeV ) considered in this search. In the absence of a full calculation, a conservative estimate of the possible size of such effects is included as a signal normalization systematic uncertainty following a parameterization as a function of $m_{H}: 150 \% \times m_{H}^{3}[\mathrm{TeV}]$, for $m_{H} \geqslant 300 \mathrm{GeV}$ [35].

The $Z Z^{(*)}$ continuum background is modelled using pythia. The mCFM [63,64] prediction, including both quark-antiquark annihilation and gluon fusion at QCD NLO, is used for the inclusive total cross section and the shape of the invariant mass of the $Z Z^{(*)}$ system $\left(m_{Z Z^{(*)}}\right)$. The QCD scale uncertainty has a $\pm 5 \%$ effect on the expected $Z Z^{(*)}$ background, and the effect due to the PDF and $\alpha_{s}$ uncertainties is $\pm 4 \%$ ( $\pm 8 \%$ ) for quark-initiated (gluoninitiated) processes. An additional theoretical uncertainty of $\pm 10 \%$ on the inclusive $Z Z^{(*)}$ cross section is conservatively included due to the missing higher-order QCD corrections for the gluoninitiated process, and a correlated uncertainty on the predicted $m_{Z Z^{(*)}}$ spectrum is estimated by varying the gluon-initiated contribution by $100 \%$ [65].

The $Z+$ jets production is modelled using alpgen [66] and is divided into two sources: $Z+$ light jets - which includes $Z c \bar{c}$ in the massless $c$-quark approximation and $Z b \bar{b}$ from parton showers - and $Z b \bar{b}$ using matrix-element calculations that take into account the $b$-quark mass. The MLM [67] matching scheme is used to remove any double counting of identical jets produced via the matrix-element calculation and the parton shower, but this scheme is not implemented for $b$-jets. Therefore, $b \bar{b}$ pairs with separation $\Delta R=\sqrt{(\Delta \phi)^{2}+(\Delta \eta)^{2}}>0.4$ between the $b$-quarks are taken from the matrix-element calculation, whereas for $\Delta R<0.4$ the partonshower $b \bar{b}$ pairs are used. In this search the $Z+$ jets background is normalized using control samples from data. For comparisons with simulation, the QCD NNLO FEWZ $[68,69]$ and MCFM cross section calculations are used for inclusive $Z$ boson and $Z b \bar{b}$ production, respectively. The $t \bar{t}$ background is modelled using mc@nlo [70] and is normalized to the approximate NNLO cross section calculated using hathor [71]. The effect of the QCD scale uncertainty on the cross section is ${ }_{-9}^{+4} \%$, while the effect of PDF and $\alpha_{s}$ uncertainties is $\pm 7 \%$. Both ALPGEN and mc@nlo are interfaced to HERWIG [72] for parton shower hadronization and to JIMMY [73] for the underlying event simulation.

Table 2
Lower thresholds applied to $m_{34}$ for reference values of $m_{4 \ell}$. For $m_{4 \ell}$ values between these reference values the selection requirement is obtained via linear interpolation.

| $m_{4 \ell}(\mathrm{GeV})$ | $\leqslant 120$ | 130 | 140 | 150 | 160 | 165 | 180 | 190 |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $m_{34}$ threshold $(\mathrm{GeV})$ | 15 | 20 | 25 | 30 | 30 | 35 | 40 | 50 |

Generated events are fully simulated using the ATLAS detector simulation [74] within the GEANT4 framework [75]. Additional $p p$ interactions in the same and nearby bunch crossings (pile-up) are included in the simulation. The MC samples are reweighted to reproduce the observed distribution of the mean number of interactions per bunch crossing in the data.

## 4. Lepton identification and event selection

The data considered in this analysis are selected using singlelepton or di-lepton triggers. For the single-muon trigger the $p_{T}$ threshold is 18 GeV , while for the single-electron trigger the transverse energy, $E_{\mathrm{T}}$, threshold is $20-22 \mathrm{GeV}$ depending on the LHC instantaneous luminosity. For the di-muon and di-electron triggers the thresholds are $p_{\mathrm{T}}=10 \mathrm{GeV}$ for each of the muons, and $E_{\mathrm{T}}=12 \mathrm{GeV}$ for each of the electrons, respectively.

Electron candidates consist of clusters of energy deposited in the electromagnetic calorimeter that are associated to ID tracks. Electron tracks have been refitted using a Gaussian-sum filter. The electron candidates must satisfy a set of identification criteria [76] that require the shower profiles to be consistent with those expected for electromagnetic showers and a well-reconstructed ID track pointing to the corresponding cluster. The electron transverse momentum is computed from the cluster energy and the track direction at the interaction point.

Muon candidates are reconstructed by matching ID tracks with either complete or partial tracks reconstructed in the MS [77]. If a complete track is present, the two independent momentum measurements are combined; otherwise the momentum is measured using the ID information only. To reject cosmic rays, muon tracks are required to have a transverse impact parameter, defined as the impact parameter in the transverse plane with respect to the primary vertex, of less than 1 mm . The primary vertex is defined as the reconstructed vertex with the highest $\sum p_{\mathrm{T}}^{2}$ of associated tracks among the reconstructed vertices with at least three associated tracks.

This analysis searches for Higgs boson candidates by selecting two same-flavour, opposite-sign lepton pairs in an event. The impact parameter of the leptons along the beam axis is required to be within 10 mm of the primary vertex. Each lepton must satisfy $p_{\mathrm{T}}>7 \mathrm{GeV}$ and be measured in the pseudorapidity range $|\eta|<2.47$ for electrons and $|\eta|<2.7$ for muons. At least two leptons in the quadruplet must have $p_{\mathrm{T}}>20 \mathrm{GeV}$. The leptons are required to be separated from each other by $\Delta R>0.1$. The invariant mass of the same-flavour and opposite-sign lepton pair closest to the $Z$ boson mass $\left(m_{Z}\right)$ is denoted by $m_{12}$ and $\left|m_{Z}-m_{12}\right|<$ 15 GeV is required. The invariant mass of the remaining sameflavour and opposite-sign lepton pair, $m_{34}$, is required to be in the range $m_{\min }<m_{34}<115 \mathrm{GeV}$, where $m_{\text {min }}$ depends on the reconstructed four-lepton invariant mass, $m_{4 \ell}$, as shown in Table 2.

The $Z+$ jets and $t \bar{t}$ background contributions are further reduced by applying track- and calorimeter-based isolation and impact parameter requirements on the leptons. For a lepton to be isolated, the sum of the $p_{\mathrm{T}}$ of tracks within $\Delta R<0.2$ of the lepton divided by the lepton $p_{\mathrm{T}}$ is required to be less than 0.15 , while the sum of the $E_{\mathrm{T}}$ of the calorimeter cells with $\Delta R<0.2$ around the lepton divided by the lepton $p_{\mathrm{T}}$ is required to be less than 0.3 . The lepton track and the energies of calorimeter cells associated to it are excluded from the sum. Any contributions arising from other
leptons of the quadruplet are subtracted. To reduce the impact of event pile-up, the tracks included in the $p_{\mathrm{T}}$ sum for track isolation must be associated with the primary vertex, and the transverse energy included in the $E_{T}$ sum for calorimeter isolation is corrected by subtracting a small amount of energy that depends on the number of reconstructed vertices in the event. In events with four-lepton invariant mass ( $m_{4 \ell}$ ) below 190 GeV , the transverse impact parameter significance, defined as the transverse impact parameter divided by the corresponding uncertainty, for the two lowest $p_{\text {T }}$ leptons in the quadruplet is required to be less than 3.5 (6) for muons (electrons).

The combined signal reconstruction and selection efficiencies for $m_{H}=130 \mathrm{GeV}\left(m_{H}=360 \mathrm{GeV}\right)$ are $27 \%(60 \%)$ for the $4 \mu$ channel, $18 \%$ ( $52 \%$ ) for the $2 e 2 \mu$ channel and $14 \%$ ( $45 \%$ ) for the $4 e$ channel. The final discriminating variable is $m_{4 \ell}$, for which Higgs boson production would appear as a clustering of events. In Fig. 1, the invariant mass distributions for the $4 \mu$ and $4 e$ channels are presented for a simulated signal sample with $m_{H}=130 \mathrm{GeV}$. The width of the reconstructed Higgs boson mass distribution is dominated by experimental resolution for $m_{H}<350 \mathrm{GeV}$, while for higher $m_{H}$ the reconstructed width is dominated by the natural width of the Higgs boson; the predicted full-width at halfmaximum is approximately 35 GeV at $m_{H}=400 \mathrm{GeV}$.

## 5. Background estimation

The expected background yield and its composition is estimated using MC simulation normalized to the theoretical cross section for $Z Z^{(*)}$ production and by data-driven methods for the $Z+$ jets and $t \bar{t}$ processes.

A control sample consisting of $Z \rightarrow \ell^{+} \ell^{-}$candidates with an additional loosely selected - no isolation or impact parameter requirements - same-flavour lepton pair is used to study the contributions of $Z b \bar{b}$ and $Z+$ light jets. The $Z b \bar{b}$ background dominates the $Z+\mu \mu$ sample, and the $Z+$ light jets background dominates in the $Z+e e$ sample. The heavy flavour contribution in the $Z+\mu \mu$ control sample is estimated by subtracting from the data the light jet component. The latter is obtained in a data-driven manner by using measurements of the rate at which other particles are misidentified as muons. The $Z+$ light jets contribution in the $Z+e e$ final state is estimated by extrapolation, using MC simulation, from a background-dominated region defined by inverting the electron identification requirement on the transverse shower shape of the electromagnetic energy deposit. These data-driven backgrounds are extrapolated to the signal region by applying the efficiencies found in MC simulation, and verified using data, for the isolation and impact parameter significance requirements.

The normalization of the $t \bar{t}$ background, which also contributes substantially in the $Z+\mu \mu$ final state, is verified using a control region of events containing an opposite-sign electron-muon pair consistent with the $Z$ boson mass and two additional same-flavour leptons.

Fig. 2 displays the invariant masses of lepton pairs in events with a $Z$ boson candidate and an additional same-flavour lepton pair, selected by following the kinematic requirements of the analysis, and by applying isolation requirements to the first lepton pair only. The events are divided according to the flavour of the additional lepton pair into $Z+\mu \mu$ and $Z+e e$ samples, where $Z \rightarrow \mu^{+} \mu^{-} / e^{+} e^{-}$. In Figs. 2(a) and 2(c) the $m_{12}$ and $m_{34}$ distribu-


Fig. 1. Invariant mass distributions for simulated (a) $H \rightarrow Z Z^{(*)} \rightarrow 4 \mu$ and (b) $H \rightarrow Z Z^{(*)} \rightarrow 4 e$ events for $m_{H}=130 \mathrm{GeV}$. The fitted range for the Gaussian is chosen to be: $-2 \sigma$ to $2 \sigma(-1.5 \sigma$ to $2.5 \sigma)$ for the $4 \mu(4 e)$ channel. The reduced mean value of the reconstructed invariant mass in the $4 e$ channel arises from energy losses due to bremsstrahlung [76]. The fraction of events outside the $\pm 2 \sigma$ region is found to be $15 \%$ for $4 \mu$ and $18 \%$ for $4 e$.
tions are presented for $Z+\mu \mu$ events, while in Figs. 2(b) and 2(d) the corresponding distributions are presented for $Z+e e$ events. The shapes and normalizations of the backgrounds discussed earlier are in good agreement with data; this is observed both for large values of $m_{34}$, where the $Z Z^{(*)}$ background dominates, and for low $m_{34}$ values.

## 6. Systematic uncertainties

Uncertainties in lepton reconstruction and identification efficiency, and on the momentum resolution and scale, are determined using samples of $W, Z$ and $J / \psi$ decays. The muon efficiency uncertainty results in a relative acceptance uncertainty in the signal and the $Z Z^{(*)}$ background which is uniform over the mass range of interest, and amounts to $0.22 \%(0.16 \%)$ for the $4 \mu(2 e 2 \mu)$ channel. The uncertainty in the electron efficiency results in a relative acceptance uncertainty of $2.3 \%$ (1.6\%) for the $4 e(2 e 2 \mu)$ channel at $m_{4 \ell}=600 \mathrm{GeV}$ and reaches $8.0 \%$ (4.1\%) at $m_{4 \ell}=110 \mathrm{GeV}$. The effects of muon momentum resolution and scale uncertainties are found to be negligible. The energy resolution uncertainty for electrons is negligible, while the electron energy scale uncertainty results in an uncertainty of less than $0.6 \%(0.3 \%)$ on the mass scale of the $m_{4 \ell}$ distribution for the $4 e(2 e 2 \mu)$ channel.

The selection efficiencies of the isolation and impact parameter requirements are studied using data for both isolated and non-isolated leptons. Isolated leptons are obtained from $Z \rightarrow \ell \ell$ decays, while additional leptons reconstructed in events with $Z \rightarrow \ell \ell$ decays constitute the sample of non-isolated leptons. Additional checks are performed with non-isolated leptons from semileptonic $b$ - and $c$-quark decays in a heavy-flavour enriched di-jet sample. Good agreement is observed between data and simulation and the systematic uncertainty is, in general, estimated to be small with respect to the other systematic uncertainties. An exception is found in the case of isolated electrons with $E_{\mathrm{T}}<15 \mathrm{GeV}$, where due to the small number of $Z \rightarrow e^{+} e^{-}$events and the substantial QCD backgrounds an additional uncertainty of $5 \%$ is added.

An additional uncertainty in the signal selection efficiency is added due to the modelling of the signal kinematics. This is evaluated by varying the Higgs boson $p_{\mathrm{T}}$ spectrum in the gluon fusion process according to the PDF and QCD scale uncertainties.

The $Z+$ light jets and $Z b \bar{b}$ backgrounds are evaluated using data. Systematic uncertainties of $45 \%$ and $40 \%$, respectively, are assigned to their normalization to account for the statistical uncertainty in the yield of the control sample, the uncertainty in the composition of the control sample, and the uncertainty in the MC-based extrapolation to the signal region.

The overall uncertainty in the integrated luminosity for the complete 2011 dataset is $3.9 \%$, based on the calibration described in Refs. [14,15] including an additional uncertainty for the extrapolation to the later data-taking period with higher instantaneous luminosity.

## 7. Results

In total, 71 candidate events are selected by the analysis: $244 \mu, 302 e 2 \mu$, and $174 e$ events. From the background processes, $62 \pm 9$ events are expected: $18.6 \pm 2.84 \mu, 29.7 \pm 4.52 e 2 \mu$ and $13.4 \pm 2.04 e$. In Table 3, the number of events observed in each final state is summarized and compared to the expected backgrounds, separately for $m_{4 \ell}<180 \mathrm{GeV}$ and $m_{4 \ell} \geqslant 180 \mathrm{GeV}$, and to the expected signal for various $m_{H}$ hypotheses. The $m_{12}$ and $m_{34}$ mass spectra are shown in Fig. 3. The expected $m_{4 \ell}$ distributions for the total background and several signal hypotheses are compared to the data in Fig. 4.

Upper limits are set on the Higgs boson production cross section at $95 \% \mathrm{CL}$, using the $C L_{s}$ modified frequentist formalism [78] with the profile likelihood ratio test statistic [79]. The test statistic is evaluated with a binned maximum-likelihood fit of signal and background models to the observed $m_{4 \ell}$ distribution. Fig. 5 shows the observed and expected $95 \%$ CL cross section upper limits, calculated using ensembles of simulated pseudo-experiments, as a function of $m_{H}$. The SM Higgs boson is excluded at $95 \% \mathrm{CL}$ in the mass ranges $134-156 \mathrm{GeV}, 182-233 \mathrm{GeV}, 256-265 \mathrm{GeV}$ and $268-415 \mathrm{GeV}$. The expected exclusion ranges are $136-157 \mathrm{GeV}$ and $184-400 \mathrm{GeV}$.

The significance of an excess is given by the probability, $p_{0}$, that a background-only experiment is more signal-like than that observed. In Fig. 6 the $p_{0}$-values, calculated using an ensemble of simulated pseudo-experiments, are given as a function of $m_{H}$ for the full mass range of the analysis. The most significant upward deviations from the background-only hypothesis are observed for


Fig. 2. Invariant mass distributions of the lepton pairs in the control sample defined by a $Z$ boson candidate and an additional same-flavour lepton pair. The sample is divided according to the flavour of the additional lepton pair. In (a) the $m_{12}$ and in (c) the $m_{34}$ distributions are presented for $Z\left(\rightarrow \mu^{+} \mu^{-} / e^{+} e^{-}\right)+\mu \mu$ events. In (b) the $m_{12}$ and in (d) the $m_{34}$ distributions are presented for $Z\left(\rightarrow \mu^{+} \mu^{-} / e^{+} e^{-}\right)+e e$ events. The kinematic selections of the analysis are applied. Isolation requirements are applied to the first lepton pair only.

Table 3
The expected numbers of background events, with their systematic uncertainty, separated into "Low- $m_{4 \ell}$ " ( $m_{4 \ell}<180 \mathrm{GeV}$ ) and "High- $m_{4 \ell}$ " ( $m_{4 \ell} \geqslant 180 \mathrm{GeV}$ ) regions, compared to the observed numbers of events. The expectations for a Higgs boson signal for five different $m_{H}$ values are also given.

|  | $\mu^{+} \mu^{-} \mu^{+} \mu^{-}$ |  | $e^{+} e^{-} \mu^{+} \mu^{-}$ |  | $e^{+} e^{-} e^{+} e^{-}$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Low-m4e | High-m4e | Low-m4e | High-m4e | Low-m4e | High-m4e |
| Int. luminosity | $4.8 \mathrm{fb}^{-1}$ |  | $4.8 \mathrm{fb}^{-1}$ |  | $4.9 \mathrm{fb}^{-1}$ |  |
| Z $\mathbf{Z}^{(*)}$ | $2.1 \pm 0.3$ | $16.3 \pm 2.4$ | $2.8 \pm 0.6$ | $25.2 \pm 3.8$ | $1.2 \pm 0.3$ | $10.4 \pm 1.5$ |
| $Z+$ jets and $t \bar{t}$ | $0.16 \pm 0.06$ | $0.02 \pm 0.01$ | $1.4 \pm 0.5$ | $0.17 \pm 0.08$ | $1.6 \pm 0.7$ | $0.18 \pm 0.08$ |
| Total background | $2.2 \pm 0.3$ | $16.3 \pm 2.4$ | $4.3 \pm 0.8$ | $25.4 \pm 3.8$ | $2.8 \pm 0.8$ | $10.6 \pm 1.5$ |
| Data | 3 | 21 | 3 | 27 | 2 | 15 |
| $m_{H}=130 \mathrm{GeV}$ | $1.00 \pm 0.17$ |  | $1.22 \pm 0.21$ |  | $0.43 \pm 0.08$ |  |
| $m_{H}=150 \mathrm{GeV}$ | $2.1 \pm 0.4$ |  | $2.9 \pm 0.4$ |  | $1.12 \pm 0.18$ |  |
| $m_{H}=200 \mathrm{GeV}$ | $4.9 \pm 0.7$ |  | $7.7 \pm 1.0$ |  | $3.1 \pm 0.4$ |  |
| $m_{H}=400 \mathrm{GeV}$ | $2.0 \pm 0.3$ |  | $3.3 \pm 0.5$ |  | $1.49 \pm 0.21$ |  |
| $m_{H}=600 \mathrm{GeV}$ | $0.34 \pm 0.04$ |  | $0.62 \pm 0.10$ |  | $0.30 \pm 0.06$ |  |

$m_{H}=125 \mathrm{GeV}$ with a local $p_{0}$ of $1.6 \%$ (2.1 standard deviations), $m_{H}=244 \mathrm{GeV}$ with a local $p_{0}$ of $1.3 \%$ (2.2 standard deviations) and $m_{H}=500 \mathrm{GeV}$ with a local $p_{0}$ of $1.8 \%$ (2.1 standard deviations). The median expected local $p_{0}$ in the presence of a SM Higgs boson are $10.6 \%$ ( 1.3 standard deviations), $0.14 \%$ ( 3.0 stan-
dard deviations) and $7.1 \%$ ( 1.5 standard deviations) for $m_{H}=$ $125 \mathrm{GeV}, 244 \mathrm{GeV}$ and 500 GeV , respectively. An alternative calculation, using the asymptotic approximation of Ref. [79], yielded compatible results - within 0.2 standard deviations - in the entire mass range.


Fig. 3. Invariant mass distributions (a) $m_{12}$ and (b) $m_{34}$ for the selected candidates. The data (dots) are compared to the background expectations from the dominant $Z Z(*)$ process and the sum of $t \bar{t}, Z b \bar{b}$ and $Z+$ light jets processes. Error bars represent $68.3 \%$ central confidence intervals.


 dominated by detector resolution at low $m_{H}$ values and by the Higgs boson width at high $m_{H}$.

The quoted values do not account for the so-called lookelsewhere effect, which takes into account that such an excess (or a larger one) can appear anywhere in the search range as a result of an upward fluctuation of the background. When considering the complete mass range of this search, using the method of Ref. [80], the global $p_{0}$-value for each of the three excesses becomes of $O(50 \%)$. Thus, once the look-elsewhere effect is considered, none of the observed local excesses are significant.

## 8. Summary

A search for the SM Higgs boson in the decay channel $H \rightarrow$ $Z Z^{(*)} \rightarrow 4 \ell$ based on $4.8 \mathrm{fb}^{-1}$ of data recorded by the ATLAS detector at $\sqrt{s}=7 \mathrm{TeV}$ during the 2011 run has been presented. The SM Higgs boson is excluded at $95 \% \mathrm{CL}$ in the mass ranges $134-156 \mathrm{GeV}, 182-233 \mathrm{GeV}, 256-265 \mathrm{GeV}$ and $268-415 \mathrm{GeV}$. The largest upward deviations from the background-only hypothesis are observed for $m_{H}=125 \mathrm{GeV}, 244 \mathrm{GeV}$ and 500 GeV with local
significances of 2.1, 2.2 and 2.1 standard deviations, respectively. Once the look-elsewhere effect is considered, none of these excesses are significant.

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Fig. 5. The expected (dashed) and observed (full line) 95\% CL upper limits on the Standard Model Higgs boson production cross section as a function of $m_{H}$, divided by the expected SM Higgs boson cross section. The dark (green) and light (yellow) bands indicate the expected limits with $\pm 1 \sigma$ and $\pm 2 \sigma$ fluctuations, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this Letter.)


Fig. 6. The observed local $p_{0}$, the probability that the background fluctuates to the observed number of events or higher, is shown as the solid line. The dashed curve shows the expected median local $p_{0}$ for the signal hypothesis when tested at $m_{H}$. The two horizontal dashed lines indicate the $p_{0}$ values corresponding to local significances of $2 \sigma$ and $3 \sigma$.

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# Search for extra dimensions using diphoton events in 7 TeV proton-proton collisions with the ATLAS detector ${ }^{\text {* }}$ 

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#### Abstract

Using data recorded in 2011 with the ATLAS detector at the Large Hadron Collider, a search for evidence of extra spatial dimensions has been performed through an analysis of the diphoton final state. The analysis uses data corresponding to an integrated luminosity of $2.12 \mathrm{fb}^{-1}$ of $\sqrt{s}=7 \mathrm{TeV}$ protonproton collisions. The diphoton invariant mass ( $m_{\gamma \gamma}$ ) spectrum is observed to be in good agreement with the expected Standard Model background. In the large extra dimension scenario of Arkani-Hamed, Dimopoulos and Dvali, the results provide $95 \%$ CL lower limits on the fundamental Planck scale between 2.27 and 3.53 TeV , depending on the number of extra dimensions and the theoretical formalism used. The results also set $95 \%$ CL lower limits on the lightest Randall-Sundrum graviton mass of between 0.79 and 1.85 TeV , for values of the dimensionless coupling $k / \bar{M}_{P l}$ varying from 0.01 to 0.1 . Combining with previously published ATLAS results from the dielectron and dimuon final states, the 95\% CL lower limit on the Randall-Sundrum graviton mass for $k / \bar{M}_{P l}=0.01$ (0.1) is 0.80 (1.95) TeV. © 2012 CERN. Published by Elsevier B.V. All rights reserved.


## 1. Introduction

The enormous difference between the Planck scale and the electroweak scale is known as the hierarchy problem. A prominent class of new physics models addresses the hierarchy problem through the existence of extra spatial dimensions. In this Letter, we search for evidence of extra dimensions within the context of the models of Arkani-Hamed, Dimopoulos, and Dvali (ADD) [1] and of Randall and Sundrum (RS) [2]. In these models, gravity can propagate in the higher-dimensional bulk, giving rise to a socalled Kaluza-Klein (KK) tower of massive spin-2 graviton excitations (KK gravitons, $G$ ). Due to their couplings to Standard Model (SM) particle-antiparticle pairs, KK gravitons can be investigated in proton-proton ( $p p$ ) collisions at the Large Hadron Collider (LHC) via a variety of processes, including virtual graviton exchange as well as direct graviton production through gluon-gluon fusion or quark-antiquark annihilation.

The ADD model [1] postulates the existence of $n$ flat additional spatial dimensions compactified with radius $R$, in which only gravity propagates. The fundamental Planck scale in the $(4+n)$ dimensional spacetime, $M_{D}$, is related to the apparent scale $M_{P l}$ by Gauss' law: $\bar{M}_{P l}^{2}=M_{D}^{n+2} R^{n}$, where $\bar{M}_{P l}=M_{P l} / \sqrt{8 \pi}$ is the reduced Planck scale. The mass splitting between subsequent KK states is of order $1 / R$. In the ADD model, resolving the hierarchy problem requires typically small values of $1 / R$, giving rise to an almost continuous spectrum of KK graviton states.

[^20]While processes involving direct graviton emission depend on $M_{D}$, effects involving virtual gravitons depend on the ultraviolet cutoff of the KK spectrum, denoted $M_{S}$. The effects of the extra dimensions are typically parametrized by $\eta_{G}=\mathcal{F} / M_{S}^{4}$, where $\eta_{G}$ describes the strength of gravity in the presence of the extra dimensions and $\mathcal{F}$ is a dimensionless parameter of order unity reflecting the dependence of virtual KK graviton exchange on the number of extra dimensions. Several theoretical formalisms exist in the literature, using different definitions of $\mathcal{F}$ and, consequently, of $M_{S}$ :
$\mathcal{F}=1 \quad(\mathrm{GRW})[3] ;$
$\mathcal{F}=\left\{\begin{array}{ll}\log \left(\frac{M_{S}^{2}}{\hat{s}}\right) & n=2, \\ \frac{2}{n-2} & n>2\end{array} \quad(\operatorname{HLZ})[4] ;\right.$
$\mathcal{F}= \pm \frac{2}{\pi} \quad$ (Hewett) [5];
where $\sqrt{\hat{\hat{S}}}$ is the center-of-mass energy of the parton-parton collision. Effects due to ADD graviton exchange would be evidenced by a non-resonant deviation from the SM background expectation. Collider searches for ADD virtual graviton effects have been performed at HERA [6], LEP [7], the Tevatron [8], and the LHC [9,10]. Recent diphoton results from CMS are the most restrictive so far, setting limits on $M_{S}$ in the range of $2.3-3.8 \mathrm{TeV}$ [10].

The RS model [2] posits the existence of a fifth dimension with "warped" geometry, bounded by two $(3+1)$-dimensional branes, with the SM fields localized on the so-called TeV brane and gravity originating on the other, dubbed the Planck brane, but capable
of propagating in the bulk. Mass scales on the TeV brane, such as the Planck mass describing the observed strength of gravity, correspond to mass scales on the Planck brane as given by $M_{D}=$ $M_{P l} e^{-k \pi r_{c}}$, where $k$ and $r_{c}$ are the curvature scale and compactification radius of the extra dimension, respectively. The observed hierarchy of scales can therefore be naturally reproduced in this model, if $k r_{c} \approx 12$ [11]. KK gravitons in this model would have a mass splitting of order 1 TeV and would appear as new resonances. The phenomenology can be described in terms of the mass of the lightest KK graviton excitation $\left(m_{G}\right)$ and the dimensionless coupling to the SM fields, $k / \bar{M}_{P l}$. It is theoretically preferred [11] for $k / \bar{M}_{P l}$ to have a value in the range from 0.01 to 0.1 . The most stringent experimental limits on RS gravitons are from the LHC. For $k / \bar{M}_{P l}=0.1, \sim 1 \mathrm{fb}^{-1}$ ATLAS results from $G \rightarrow e e / \mu \mu$ exclude gravitons below 1.63 TeV [12], assuming leading order (LO) cross section predictions, and a recent $2.2 \mathrm{fb}^{-1} G \rightarrow \gamma \gamma$ result from CMS excludes gravitons below 1.84 TeV [10], using next-to-leading order (NLO) cross section values. These results have surpassed the limits from searches at the Tevatron [13] and earlier searches at the LHC [14].

The diphoton final state provides a sensitive channel for this search due to the clean experimental signature, excellent diphoton mass resolution, and modest backgrounds, as well as a branching ratio for graviton decay to diphotons that is twice the value of that for graviton decay to any individual charged-lepton pair. In this Letter, we report on a search in the diphoton final state for evidence of extra dimensions, using a data sample corresponding to an integrated luminosity of $2.12 \mathrm{fb}^{-1}$ of $\sqrt{s}=7 \mathrm{TeV} p p$ collisions, recorded during 2011 with the ATLAS detector at the LHC. The measurement of the diphoton invariant mass spectrum is interpreted in both the ADD and RS scenarios.

## 2. The ATLAS detector

The ATLAS detector [15] is a multipurpose particle physics instrument with a forward-backward symmetric cylindrical geometry and near $4 \pi$ solid angle coverage. ${ }^{1}$ Closest to the beamline are tracking detectors to measure the trajectories of charged particles, including layers of silicon-based detectors as well as a transition radiation tracker using straw-tube technology. The tracker is surrounded by a thin solenoid that provides a 2 T magnetic field for momentum measurements. The solenoid is surrounded by a hermetic calorimeter system, which is particularly important for this analysis. A system of liquid-argon (LAr) sampling calorimeters is divided into a central barrel calorimeter and two endcap calorimeters, each housed in a separate cryostat. Fine-grained LAr electromagnetic (EM) calorimeters, segmented in three longitudinal layers, are used to precisely measure the energies of electrons, positrons and photons for $|\eta|<3.2$. Most of the EM shower energy is collected in the second layer, which has a granularity of $\Delta \eta \times \Delta \phi=0.025 \times 0.025$. The first layer is segmented into eight strips per middle-layer cell in the $\eta$ direction, extending over four middle-layer cells in $\phi$, designed to separate photons from $\pi^{0}$ mesons. A presampler, covering $|\eta|<1.81$, is used to correct for energy lost upstream of the calorimeter. The regions spanning $1.5<|\eta|<4.9$ are instrumented with LAr calorimetry also for hadronic measurements, while an iron-scintillator tile calorimeter provides hadronic coverage in the range $|\eta|<1.7$. A muon spectrometer consisting of three superconducting toroidal magnet

[^21]systems, tracking chambers, and detectors for triggering lies outside the calorimeter system.

## 3. Trigger and data selection

The analysis uses data collected between March and September 2011 during stable beam periods of $7 \mathrm{TeV} p p$ collisions. Selected events had to satisfy a trigger requiring at least two photon candidates with transverse energy $E_{\mathrm{T}}^{\gamma}>20 \mathrm{GeV}$ and satisfying a set of requirements, referred to as the "loose" photon definition [16], which includes requirements on the leakage of energy into the hadronic calorimeter as well as on variables that require the transverse width of the shower, measured in the second EM calorimeter layer, be consistent with the narrow width expected for an EM shower. The loose definition is designed to have high photon efficiency, albeit with reduced background rejection. The trigger was essentially fully efficient for high mass diphoton events passing the final selection requirements.

Events were required to have at least one primary collision vertex, with at least three reconstructed tracks. Selected events had to have at least two photon candidates, each with $E_{\mathrm{T}}^{\gamma}>25 \mathrm{GeV}$ and pseudorapidity $\left|\eta^{\gamma}\right|<2.37$, with the exclusion of $1.37<$ $\left|\eta^{\gamma}\right|<1.52$, the transition region between the barrel and endcap calorimeters. As described in more detail in Ref. [16], photon candidates included those classified as unconverted photons, with no associated track, or photons which converted to electron-positron pairs, with one or two associated tracks. The two photons were required to satisfy several quality criteria and to lie outside detector regions where their energy was not measured in an optimal way. The two photon candidates each had to satisfy a set of stricter requirements, referred to as the "tight" photon definition [16], which included a more stringent selection on the shower width in the second EM layer and additional requirements on the energy distribution in the first EM calorimeter layer. The tight photon definition was designed to increase the purity of the photon selection sample by rejecting most of the remaining jet background, including jets with a leading neutral hadron (mostly $\pi^{0}$ mesons) that decay to a pair of collimated photons.

The isolation transverse energy $E_{\mathrm{T}}^{i s o}$ for each photon was calculated [16] by summing over the cells of both the EM and hadronic calorimeters that surround the photon candidate within an angular cone of radius $\Delta R=\sqrt{\left(\eta-\eta^{\gamma}\right)^{2}+\left(\phi-\phi^{\gamma}\right)^{2}}<0.4$, after removing a central core that contains most of the energy of the photon. To reduce the jet background further, an isolation requirement was applied, requiring that each of the two leading photons satisfied $E_{\mathrm{T}}^{i \text { is }}<5 \mathrm{GeV}$. An out-of-core energy correction was applied, to make $E_{\mathrm{T}}^{\text {iso }}$ essentially independent of $E_{\mathrm{T}}^{\gamma}$. An ambient energy correction, based on the measurement of low transverse momentum jets [17], was also applied, on an event-by-event basis, to remove the contributions from the underlying event and from "pileup", which results from the presence of multiple $p p$ collisions within the same or nearby bunch crossings.

For events with more than two photon candidates passing all the selection requirements, the two photons with the highest $E_{\mathrm{T}}^{\gamma}$ values were considered. The diphoton invariant mass had to exceed 140 GeV . A total of 6846 events were selected.

## 4. Monte Carlo simulation studies

Monte Carlo (MC) simulations were performed to study the detector response for various possible signal models, as well as to perform some SM background studies. All MC events were simulated [18] with the ATLAS detector simulation based on geant 4 [19] and using ATLAS parameter tunes [20], and were processed through the same reconstruction software chain as used
for the data. The MC events were reweighted to mimic the pileup conditions observed in the data.

SM diphoton production was simulated with PYTHIA [21] version 6.424 and MRST2007LOMOD [22] parton distribution functions (PDFs). The PYTHIA events were reweighted as a function of diphoton invariant mass to the differential cross section predicted by the NLO calculation of DIPHOX [23] version 1.3.2. The reweighting factor varied from $\approx 1.6$ for a diphoton mass of 140 GeV , decreasing smoothly to unity for large masses. For the DIPHOX calculation, the renormalization scale and the initial and final factorization scales of the model were all set to the diphoton mass. The various scales were varied by a factor of two both up and down, compared to this central value, to evaluate systematic uncertainties. The PDFs were chosen following the recommendations of the PDF4LHC working group [24], with MSTW2008 NLO PDFs [25] used for the NLO predictions, and CTEQ6.6 [26] and MRST2007LOMOD [22] used for systematic comparisons.

SHERPA [27] version 1.2.3 was used with CTEQ6L [26] PDFs to simulate the various ADD scenarios for a variety of $M_{S}$ values. Due to the interference between the SM and gravity-mediated contributions, it is necessary to simulate events according to the full differential cross section as a function of the diphoton mass. A generator-level cut was applied to restrict the signal simulation to diphoton masses above 200 GeV . The ADD MC samples were used to determine the signal acceptance ( $A$ ) and selection efficiency $(\epsilon)$. The acceptance, defined as the percentage of diphoton signal events with the two highest $E_{\mathrm{T}}$ photons passing the applied $E_{\mathrm{T}}^{\gamma}$ and $\eta^{\gamma}$ cuts, varied somewhat for the various ADD implementations and fell from typical values of $\approx 20 \%$ for $M_{S}=1.5 \mathrm{TeV}$ down to $\approx 15 \%$ for $M_{S}=3 \mathrm{TeV}$, due mostly to the variations in the $\eta^{\gamma}$ distributions. The selection efficiency, for events within the detector acceptance, was found to be $\approx 70 \%$.

RS model MC signal samples were produced using the implementation of the RS model in PYTHIA [21] version 6.424, which is fully specified by providing the values of $m_{G}$ and $k / \bar{M}_{P l}$. MC signal samples were produced for a range of $m_{G}$ and $k / \bar{M}_{P l}$ values, using the MRST2007LOMOD [22] PDFs. The products of $A \times \epsilon$ for the RS signal models were in the range $\approx(53-60) \%$, slowly rising with increasing graviton mass. The reconstructed shape of the graviton resonance was modeled by convolving the graviton BreitWigner lineshape with a double-sided Crystal Ball (CB) function to describe the detector response. The natural width of the BreitWigner was fixed according to the expected theoretical value, which varies as the square of $k / \bar{M}_{P l}$. The values of the width increase, for $k / \bar{M}_{P l}=0.1$, from $\approx 8 \mathrm{GeV}$ up to $\approx 30 \mathrm{GeV}$ for $m_{G}$ values from 800 GeV to 2200 GeV , respectively. The parameters of the CB function, which includes a Gaussian core to model the detector resolution matched to exponential functions on both sides to model the modest non-Gaussian tails, were determined by fitting to the reconstructed MC signals. The fitted values of $\sigma$ of the Gaussian core approached a value of $\approx 1 \%$ for high $m_{G}$ values, as expected given the current value of the constant term in the EM calorimeter energy resolution, and were found to be independent of $k / \bar{M}_{P l}$. The EM energy resolution has been verified in data using $Z \rightarrow e e$ decays [28], and MC used to describe the modest differences between the response to photons versus electrons. The fitted values of the CB parameters varied smoothly with $m_{G}$. Fitting this mass dependence provided a signal parametrization that was used to describe signals with any values of $m_{G}$ and $k / \bar{M}_{P l}$.

## 5. Background evaluation

The largest background for this analysis is the irreducible background due to SM $\gamma \gamma$ production. The shape of the diphoton invariant mass spectrum from this background was estimated using

MC, reweighting the PYTHIA samples to the differential cross section predictions of DIPHOX.

Another significant background component is the reducible background that includes events in which one or both of the reconstructed photon candidates result from a different physics object being misidentified as a photon. This background is dominated by $\gamma+$ jet $(j)$ and $j j$ events, with one or two jets faking photons, respectively. Backgrounds with electrons faking photons, such as the Drell-Yan production of electron-positron pairs as well as $W / Z+\gamma$ and $t \bar{t}$ processes, were verified using MC to be small after the event selection and were neglected. Several backgroundenriched control samples were defined in order to determine the shape of the reducible background using data-driven techniques. In all control samples, the two photon candidates were required to pass the same isolation cut as for the signal selection, since removing the isolation requirement was seen to modify the diphoton mass spectrum. The first control sample contained those events where one of the photon candidates passed the tight requirement applied for the signal selection. However, the other photon candidate was required to fail the tight photon identification definition, but to pass the loose requirement; the latter restriction was applied to avoid any trigger bias, as the trigger required two loose photons. This sample is enriched in $\gamma+j$ events, where the photon passed the tight requirement and a jet passed the loose one, and also in $j j$ events where both photon candidates were due to jets. A second control sample, dominated by $j j$ events, was similarly defined, but both photon candidates were required to fail the tight photon identification while passing the loose definition.

The diphoton invariant mass distributions were compared for these control samples. To check for any kinematic bias, the control sample with one tight and one loose photon candidate was further divided, with the $\gamma j(j \gamma)$ subsample being defined as the case with the tight photon being the photon candidate with the highest (second highest) transverse energy. The diphoton invariant mass distributions of all three control subsamples were found to be consistent with each other, within statistical uncertainties. The sum of the control samples was used to provide the best estimate of the reducible background shape. Variations among the subsamples were taken into account as a source of systematic uncertainty in the reducible background prediction.

The data control samples have relatively few events in the high diphoton mass signal region. It was therefore necessary to extrapolate the reducible background shape to higher masses, which was done by fitting with a smooth function of the form $f(x)=$ $p_{1} \times x^{p_{2}+p_{3} \log x}$, where $x=m_{\gamma \gamma}$ and $p_{i}$ are the fit parameters. This functional form has been used in previous ATLAS resonance searches [12,29], and describes well the shape of the control data samples.

The total background, calculated as the sum of the irreducible and reducible components, was normalized to the number of data events in a low mass control region with diphoton masses between 140 and 400 GeV , in which possible ADD and RS signals have been excluded by previous searches. The fraction of the total background in this region that is due to the irreducible background is defined as the purity of the sample. The purity $(p)$ was determined by three complementary methods. The most precise measurement resulted from a method previously used in Refs. $[30,31]$ that examines the $E_{\mathrm{T}}^{\text {iso }}$ values of the two photon candidates. Templates for the $E_{\mathrm{T}}^{\text {iso }}$ distributions of true photons and of fake photons from jets were both determined from the data. The shape for fake photons was found using a sample of photon candidates that failed at least one of a subset of several of the selection requirements used for the tight photon definition. The shape for photons was found from the tight photon sample, after subtracting the fake photon shape normalized to match the number of candidates with large
values (greater than 10 GeV ) of $E_{\mathrm{T}}^{\text {iso }}$. In addition, for $j j$ events, due to the observed significant ( $\approx 20 \%$ ) correlation between the $E_{\mathrm{T}}^{\text {iso }}$ values of the two photon candidates, a two-dimensional template was formed using events in which both photon candidates failed the tight identification. An extended maximum likelihood fit to the two-dimensional distribution formed from the $E_{\mathrm{T}}^{\text {iso }}$ values of the two photon candidates was performed in order to extract the contributions from $\gamma \gamma, \gamma j, j \gamma$, and $j j$ events. The fit was performed using the photon and fake photon $E_{\mathrm{T}}^{i s o}$ templates, as well as the two-dimensional $j j$ template. The resultant value of the purity in the low mass control region was $p=71_{-9}^{+5} \%$. The uncertainty was determined by varying the subset of tight selection criteria failed by fake photon candidates, and then repeating the purity determination. Cross checks using either the DIPHOX prediction for the absolute normalization of the irreducible component, or fitting the shapes of the irreducible and reducible backgrounds to the data in the low mass control region, yielded consistent, but less precise results. The result from the isolation method was therefore used as the best estimate of the purity, and the total SM background prediction was set equal to the sum of the irreducible and reducible components, weighted appropriately by this purity value and normalized to data in the low mass control region.

## 6. Systematic uncertainties

Systematic uncertainties in the DIPHOX prediction for the shape of the irreducible background were obtained by varying the scales of the model and the PDFs, while keeping the overall normalization fixed in the low mass control region in which the total background prediction was normalized to the data. The resultant systematic uncertainties range from a few percent at low masses, up to $\approx 15 \%$ for diphoton masses of $\approx 2 \mathrm{TeV}$. Systematic uncertainties in the reducible background shape were obtained by comparing the results of the extrapolation fit for the various control data subsamples, in each case maintaining the overall normalization to the data in the low mass control region. The resultant uncertainties increase from $\approx 5 \%$ for low masses to $\approx 100 \%$ at a mass of $\approx 2 \mathrm{TeV}$.

The systematic uncertainty on the shape of the total background was obtained by adding in quadrature the uncertainties on the shapes of the irreducible and reducible background components, weighted appropriately to account for the purity. In addition, there is a contribution, which is roughly constant with a value of $\approx 10 \%$ for diphoton masses above 800 GeV , introduced by varying the purity value within its uncertainty. An additional overall uncertainty of $\approx 2 \%$ was included due to the finite statistics of the data sample in the low mass control region.

The total background systematic uncertainty starts at $\approx 2 \%$ for $m_{\gamma \gamma}=140 \mathrm{GeV}$, rises to $\approx 15 \%$ by 700 GeV and then increases slowly up to almost $20 \%$ for the highest $m_{\gamma \gamma}$ values, above 2 TeV.

Systematic uncertainties on the signal yields were evaluated separately for the ADD and RS models. Since the differences were small, for simplicity the higher value was taken and applied to both models. The systematic uncertainties considered for the signal yield include the $3.7 \%$ uncertainty on the integrated luminosity [32], and a $1 \%$ uncertainty to account for the limited signal MC statistics. A value of $1 \%$ for the uncertainty on the bunch crossing identification (BCID) efficiency accounts for the ability of the Level 1 trigger hardware to pick the correct BCID when signal pulse saturation occurs in the trigger digitization. In addition, a value of $2 \%$ was applied for the uncertainty on the efficiency of the diphoton trigger. An uncertainty of $2.5 \%$ was applied due to the influence of pileup on the signal efficiency. Finally, a value of
4.3\% was taken to account for the uncertainty in the selection and identification of the pair of photons, including uncertainties due to the photon isolation cut, the description of the detector material, the tight photon identification requirements, and extrapolation to the high photon $E_{\mathrm{T}}$ values typical of the signal models. Uncertainties due to the current knowledge of the EM energy scale and resolution were verified to have a negligible impact. Adding all effects in quadrature, the total systematic uncertainty on the signal yields was 6.7\%.

Uncertainties in the theoretical signal cross sections due to PDFs and due to the NLO approximation were considered. The uncertainties due to PDFs range from $\approx 10-15 \%$ for ADD models and from $\approx 5-10 \%$ for RS models. The authors of Refs. [33,34] have privately updated their calculations of the NLO signal cross sections for 14 TeV , and provided k-factors to the LHC experiments to scale from LO to NLO cross section values for the case of 7 TeV $p p$ collisions. The NLO k-factor values, evaluated in our case for $\left|\eta^{\gamma}\right|<2.5$, have some modest dependence on the diphoton mass as well as on $M_{S}$ for the ADD model, and on the $k / \bar{M}_{P l}$ value for the RS model. However, the variations are within the theoretical uncertainty. For simplicity, therefore, constant values of 1.70 and 1.75 were assumed for the ADD and RS models, respectively, and an uncertainty in the $k$-factor value of $\pm 0.1$ was assigned to account for the variations.

## 7. Results and interpretation

Fig. 1 shows the observed invariant mass distribution of diphoton events, with the predicted SM background superimposed as well as ADD and RS signals for certain choices of the model parameters. The reducible background component is shown separately, in addition to the total background expectation, which sums the reducible and irreducible contributions. The shaded bands around each contribution indicate the corresponding uncertainty. The bottom plot of Fig. 1 shows the statistical significance, measured in standard deviations and based on Poisson distributions, of the difference between the data and the expected background in each bin. The significance was calculated and displayed as detailed in Ref. [35], and plotted as positive (negative) where there was an excess (deficit) in the data in a given bin. Table 1 lists, in bins of diphoton mass, the expected numbers of events for the irreducible and reducible background components, as well as for the total background, and also the numbers of observed data events. Both Fig. 1 and Table 1 demonstrate that there is agreement between the observed mass distribution and the expectation from the SM backgrounds over the entire diphoton mass range; no evidence is seen for either resonant or non-resonant deviations which would indicate the presence of a signal due to new physics. An analysis using the BUMPHUNTER [36] tool found that the probability, given the background-only hypothesis, of observing discrepancies at least as large as observed in the data was 0.28 , indicating quantitatively the good agreement between the data and the expected SM background.

Given the absence of evidence for a signal, 95\% CL upper limits were determined on the ADD and RS signal cross sections, using a Bayesian approach [37] with a flat prior on the signal cross section. The systematic uncertainties were incorporated as Gaussian-distributed nuisance parameters and integrated over.

To set limits on the ADD model, the number of observed events with diphoton invariant mass in a high mass signal region was compared with the expected total SM background. To optimise the expected limit, the ADD signal search region was chosen as $m_{\gamma \gamma}>1.1 \mathrm{TeV}$. There are 2 observed events in this signal region, with a background expectation of $1.33 \pm 0.26$ events,


Fig. 1. The observed invariant mass distribution of diphoton events, superimposed with the predicted SM background and expected signals for ADD and RS models with certain choices of parameters. The bin width is constant in $\log \left(m_{\gamma \gamma}\right)$. The bin-by-bin significance of the difference between data and background is shown in the lower panel.

Table 1
The expected numbers of events for the irreducible and reducible background components and for the total background, as well as the numbers of observed data events, in different diphoton mass bins. The first row, with masses from 140 to 400 GeV , corresponds to the control region in which the total background was normalized to the corresponding number of observed events. The errors include both statistical and systematic uncertainties. The errors on the irreducible and reducible background components do not include the contribution, which is anti-correlated between the two background components, from the uncertainty on the purity. However, this contribution is included in the errors listed for the total background.

| Mass range <br> $(\mathrm{GeV})$ | Background expectation |  | Observed <br> events |  |
| :--- | :---: | ---: | ---: | :---: |
|  | Irreducible | Reducible |  |  |
| $[140,400]$ | $4738 \pm 180$ | $1935 \pm 97$ | 6674 | 6674 |
| $[400,500]$ | $90.0 \pm 8.5$ | $19.9 \pm 1.8$ | $109.9 \pm 9.2$ | 102 |
| $[500,600]$ | $31.1 \pm 4.0$ | $5.8 \pm 0.8$ | $37.0 \pm 4.2$ | 36 |
| $[600,700]$ | $13.7 \pm 2.3$ | $2.0 \pm 0.4$ | $15.7 \pm 2.4$ | 16 |
| $[700,800]$ | $6.2 \pm 1.2$ | $0.8 \pm 0.2$ | $6.9 \pm 1.3$ | 9 |
| $[800,900]$ | $3.1 \pm 0.4$ | $0.3 \pm 0.1$ | $3.4 \pm 0.5$ | 5 |
| $[900,1000]$ | $1.6 \pm 0.2$ | $0.14 \pm 0.05$ | $1.8 \pm 0.3$ | 1 |
| $[1000,1100]$ | $1.0 \pm 0.2$ | $0.07 \pm 0.03$ | $1.0 \pm 0.2$ | 1 |
| $[1100,1200]$ | $0.50 \pm 0.09$ | $0.03 \pm 0.02$ | $0.54 \pm 0.11$ | 0 |
| $[1200,1300]$ | $0.29 \pm 0.07$ | $0.02 \pm 0.01$ | $0.31 \pm 0.07$ | 0 |
| $[1300,1400]$ | $0.14 \pm 0.04$ | $0.010 \pm 0.005$ | $0.15 \pm 0.04$ | 1 |
| $[1400,1500]$ | $0.13 \pm 0.04$ | $0.005 \pm 0.003$ | $0.14 \pm 0.04$ | 1 |
| $>1500$ | $0.18 \pm 0.09$ | $0.009 \pm 0.006$ | $0.19 \pm 0.09$ | 0 |

where the uncertainty includes both statistical and systematic errors. The observed (expected) 95\% CL upper limit is 2.49 (1.94) fb for the product of the cross section due to new physics multiplied by the acceptance and efficiency. The cross section result can be translated into limits on $\eta_{G}$ and, subsequently, on the parameter $M_{S}$ of the ADD model. As summarized in Table 2, assuming a k-factor of 1.70 , the $95 \%$ CL lower limits on $M_{S}$ range between 2.27 and 3.53 TeV , depending on the number of extra dimensions assumed and the ADD model implementation. LO results are also included in Table 2, for reference.

To determine the limits on the RS model, the observed invariant mass distribution was compared to templates of the expected backgrounds and varying amounts of signal for various graviton masses and $k / \bar{M}_{P l}$ values. A likelihood function was defined as the product of the Poisson probabilities over all mass bins in the

Table 2
95\% CL limits on the value of $M_{S}$ (in TeV) for various implementations of the ADD model, using both LO $(\mathrm{k}$-factor $=1)$ and NLO ( k -factor $=1.70$ ) theory cross section calculations.

| k-Factor value | GRW | Hewett |  | HLZ |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | Pos | Neg | $n=3$ | $n=4$ | $n=5$ | $n=6$ | $n=7$ |
| 1 | 2.73 | 2.44 | 2.16 | 3.25 | 2.73 | 2.47 | 2.30 | 2.17 |
| 1.70 | 2.97 | 2.66 | 2.27 | 3.53 | 2.97 | 2.69 | 2.50 | 2.36 |

Table 3
95\% CL lower limits on the mass ( GeV ) of the lightest RS graviton, for various values of $k / \bar{M}_{P I}$. The results are shown for the diphoton channel alone and for the combination of the diphoton channel with the dilepton results of Ref. [12], using both LO ( $k$-factor $=1$ ) and NLO ( $k$-factor $=1.75$ ) theory cross section calculations.

| k-Factor value | Channel(s) used | $95 \%$ CL limit $[\mathrm{TeV}]$ |  |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
|  |  |  | $k / \bar{M}_{P l}$ value |  |  |
|  |  | 0.01 | 0.03 | 0.05 | 0.1 |
| 1 | $G \rightarrow \gamma \gamma$ | 0.74 | 1.26 | 1.41 | 1.79 |
| 1.75 | $G \rightarrow \gamma \gamma / e e / \mu \mu$ | 0.76 | 1.32 | 1.47 | 1.90 |
|  |  |  |  |  |  |
|  | $G \rightarrow \gamma \gamma$ | 0.79 | 1.30 | 1.45 | 1.85 |
|  | $G \rightarrow \gamma \gamma / e e / \mu \mu$ | 0.80 | 1.37 | 1.55 | 1.95 |

search region, defined as $m_{\gamma \gamma}>500 \mathrm{GeV}$, where the Poisson probability in each bin was evaluated for the observed number of data events given the expectation from the template. The total signal acceptance as a function of mass was propagated into the expectation. The theory uncertainties were not included in the limit calculation, but are indicated by showing the theory prediction as a band with a width equal to the combined theory uncertainty when plotting the results. The resultant limits are summarized in Table 3. Using a constant k-factor value of 1.75 , the $95 \%$ CL lower limits from the diphoton channel are $m_{G}>0.79$ (1.85) TeV for $k / \bar{M}_{P l}=0.01$ (0.1).

The RS model results can be combined with the previously published ATLAS results [12] from the dilepton final state, where, assuming LO cross sections and $k / \bar{M}_{P l}=0.1$, RS gravitons with masses below 1.51 (1.45) TeV were excluded at $95 \% \mathrm{CL}$ using data samples of $1.08(1.21) \mathrm{fb}^{-1}$ to search for $G \rightarrow e e(G \rightarrow \mu \mu)$. To ensure their statistical independence, the selection cuts of the diphoton analysis included a veto of any events which were also selected by the $1.08 \mathrm{fb}^{-1} G \rightarrow e e$ analysis. In performing the combination, correlations were considered between the systematic uncertainties in the $\gamma \gamma$ and ee channels. In the ee analysis [12], the background prediction was normalized such that the expected and observed numbers of events in the region of the $Z$ peak agreed, eliminating the dependence of the ee result on the measured integrated luminosity. Therefore, the $\gamma \gamma$ and ee signal predictions were treated as uncorrelated, since there should be no correlation in the luminosity and efficiency uncertainties. The systematic uncertainty on the QCD dijet background was treated as being correlated; however, this background was quite small so the effect was minor. The PDF and scale uncertainties were treated as correlated across all three channels, and affect the irreducible background in the $\gamma \gamma$ channel as well as the Drell-Yan background in the ee/ $\mu \mu$ channels. The left plot of Fig. 2 shows the combined 95\% CL upper limit on the product of the graviton production cross section times the branching ratio for $G \rightarrow \gamma \gamma / e e / \mu \mu$, obtained using the same k -factor value of 1.75 for all three channels. As summarized in Table 3, the combined 95\% CL lower limit is $m_{G}>0.80$ (1.95) TeV for $k / \bar{M}_{P l}=0.01$ (0.1). As shown in the right plot of Fig. 2, the results can be translated into a $95 \%$ CL exclusion in the plane of $k / \bar{M}_{P l}$ versus graviton mass.


Fig. 2. (Left) Expected and observed $95 \%$ CL limits from the combination of $G \rightarrow \gamma \gamma / e e / \mu \mu$ channels on $\sigma B$, the product of the RS graviton production cross section and the branching ratio for graviton decay via $G \rightarrow \gamma \gamma / e e / \mu \mu$, as a function of the graviton mass. The theory curves are drawn assuming a k-factor of 1.75 . The thickness of the theory curve for $k / \bar{M}_{P l}=0.1$ illustrates the theoretical uncertainties. (Right) The RS results interpreted in the plane of $k / \bar{M}_{P l}$ versus graviton mass, and including recent results from other experiments [13,10]. The region above the curve is excluded at $95 \% \mathrm{CL}$. In both figures, linear interpolations are performed between the discrete set of mass points for which the dilepton limits were calculated in Ref. [12].

## 8. Summary

Using a dataset corresponding to $2.12 \mathrm{fb}^{-1}$, an analysis of the diphoton final state was used to set $95 \%$ CL lower limits of between 2.27 and 3.53 TeV on the parameter $M_{S}$ of the ADD large extra dimension scenario, depending on the number of extra dimensions and the theoretical formalism used. The diphoton results also exclude at $95 \%$ CL RS graviton masses below 0.79 (1.85) TeV for the dimensionless RS coupling $k / \bar{M}_{P l}=0.01$ (0.1). Combining with the previous ATLAS dilepton analyses further tightens these limits to exclude at $95 \%$ CL RS graviton masses below 0.80 (1.95) TeV for $k / \bar{M}_{P l}=0.01$ (0.1).

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## ATLAS Collaboration

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A. Gonidec ${ }^{29}$, S. Gonzalez ${ }^{172}$, S. González de la $\mathrm{Hoz}^{167}$, G. Gonzalez Parra ${ }^{11}$, M.L. Gonzalez Silva ${ }^{26}$, S. Gonzalez-Sevilla ${ }^{49}$, J.J. Goodson ${ }^{148}$, L. Goossens ${ }^{29}$, P.A. Gorbounov ${ }^{95}$, H.A. Gordon ${ }^{24}$, I. Gorelov ${ }^{103}$, G. Gorfine ${ }^{174}$, B. Gorini ${ }^{29}$, E. Gorini ${ }^{72 a, 72 b}$, A. Gorišek ${ }^{74}$, E. Gornicki ${ }^{38}$, S.A. Gorokhov ${ }^{128}$, V.N. Goryachev ${ }^{128}$, B. Gosdzik ${ }^{41}$, M. Gosselink ${ }^{105}$, M.I. Gostkin ${ }^{65}$, I. Gough Eschrich ${ }^{163}$, M. Gouighri ${ }^{135 a}$, D. Goujdami ${ }^{135 c}$, M.P. Goulette ${ }^{49}$, A.G. Goussiou ${ }^{138}$, C. Goy ${ }^{4}$, S. Gozpinar ${ }^{22}$, I. Grabowska-Bold ${ }^{37}$, P. Grafström ${ }^{29}$, K-J. Grahn ${ }^{41}$, F. Grancagnolo ${ }^{72 a}$, S. Grancagnolo ${ }^{15}$, V. Grassi ${ }^{148}$, V. Gratchev ${ }^{121}$, N. Grau ${ }^{34}$, H.M. Gray ${ }^{29}$, J.A. Gray ${ }^{148}$, E. 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Hassani ${ }^{136}$, M. Hatch ${ }^{29}$, D. Hauff ${ }^{99}$, S. Haug ${ }^{16}$, M. Hauschild ${ }^{29}$, R. Hauser ${ }^{88}$, M. Havranek ${ }^{20}$, B.M. Hawes ${ }^{118}$, C.M. Hawkes ${ }^{17}$, R.J. Hawkings ${ }^{29}$, A.D. Hawkins ${ }^{79}$, D. Hawkins ${ }^{163}$, T. Hayakawa ${ }^{67}$, T. Hayashi ${ }^{160}$, D. Hayden ${ }^{76}$, H.S. Hayward ${ }^{73}$, S.J. Haywood ${ }^{129}$, E. Hazen ${ }^{21}$, M. He ${ }^{\text {32d }}$, S.J. Head ${ }^{17}$, V. Hedberg ${ }^{79}$, L. Heelan ${ }^{7}$, S. Heim ${ }^{88}$, B. Heinemann ${ }^{14}$, S. Heisterkamp ${ }^{35}$, L. Helary ${ }^{4}$, C. Heller ${ }^{98}$, M. Heller ${ }^{29}$, S. Hellman ${ }^{146 a, 146 \mathrm{~b}}$, D. Hellmich ${ }^{20}$, C. Helsens ${ }^{11}$, R.C.W. Henderson ${ }^{71}$, M. Henke ${ }^{58 \mathrm{a}}$, A. Henrichs ${ }^{54}$, A.M. Henriques Correia ${ }^{29}$, S. Henrot-Versille ${ }^{115}$, F. Henry-Couannier ${ }^{83}$, C. Hensel ${ }^{54}$, T. Hen $\beta^{174}$, C.M. Hernandez ${ }^{7}$, Y. 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# Observation of a new particle in the search for the Standard Model Higgs boson with the ATLAS detector at the LHC ${ }^{\text {* }}$ 

## ATLAS Collaboration*

This paper is dedicated to the memory of our ATLAS colleagues who did not live to see the full impact and significance of their contributions to the experiment.

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#### Abstract

A search for the Standard Model Higgs boson in proton-proton collisions with the ATLAS detector at the LHC is presented. The datasets used correspond to integrated luminosities of approximately $4.8 \mathrm{fb}^{-1}$ collected at $\sqrt{s}=7 \mathrm{TeV}$ in 2011 and $5.8 \mathrm{fb}^{-1}$ at $\sqrt{s}=8 \mathrm{TeV}$ in 2012. Individual searches in the channels $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow \gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ in the 8 TeV data are combined with previously published results of searches for $H \rightarrow Z Z^{(*)}, W W^{(*)}, b \bar{b}$ and $\tau^{+} \tau^{-}$in the 7 TeV data and results from improved analyses of the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$ channels in the 7 TeV data. Clear evidence for the production of a neutral boson with a measured mass of $126.0 \pm 0.4$ (stat) $\pm 0.4$ (sys) GeV is presented. This observation, which has a significance of 5.9 standard deviations, corresponding to a background fluctuation probability of $1.7 \times 10^{-9}$, is compatible with the production and decay of the Standard Model Higgs boson.


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## 1. Introduction

The Standard Model (SM) of particle physics [1-4] has been tested by many experiments over the last four decades and has been shown to successfully describe high energy particle interactions. However, the mechanism that breaks electroweak symmetry in the SM has not been verified experimentally. This mechanism [5-10], which gives mass to massive elementary particles, implies the existence of a scalar particle, the SM Higgs boson. The search for the Higgs boson, the only elementary particle in the SM that has not yet been observed, is one of the highlights of the Large Hadron Collider [11] (LHC) physics programme.

Indirect limits on the SM Higgs boson mass of $m_{H}<158 \mathrm{GeV}$ at $95 \%$ confidence level (CL) have been set using global fits to precision electroweak results [12]. Direct searches at LEP [13], the Tevatron [14-16] and the LHC [17,18] have previously excluded, at $95 \%$ CL, a SM Higgs boson with mass below 600 GeV , apart from some mass regions between 116 GeV and 127 GeV .

Both the ATLAS and CMS Collaborations reported excesses of events in their 2011 datasets of proton-proton ( $p p$ ) collisions at centre-of-mass energy $\sqrt{s}=7 \mathrm{TeV}$ at the LHC, which were compatible with SM Higgs boson production and decay in the mass region $124-126 \mathrm{GeV}$, with significances of 2.9 and 3.1 standard deviations $(\sigma)$, respectively $[17,18]$. The CDF and $\mathrm{D} \varnothing$ experiments at the Tevatron have also recently reported a broad excess in the mass region

120-135 GeV; using the existing LHC constraints, the observed local significances for $m_{H}=125 \mathrm{GeV}$ are $2.7 \sigma$ for CDF [14], 1.1 $\sigma$ for $\mathrm{D} \emptyset$ [15] and $2.8 \sigma$ for their combination [16].

The previous ATLAS searches in $4.6-4.8 \mathrm{fb}^{-1}$ of data at $\sqrt{s}=$ 7 TeV are combined here with new searches for $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell,{ }^{1}$ $H \rightarrow \gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ in the $5.8-5.9 \mathrm{fb}^{-1}$ of $p p$ collision data taken at $\sqrt{s}=8 \mathrm{TeV}$ between April and June 2012.

The data were recorded with instantaneous luminosities up to $6.8 \times 10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$; they are therefore affected by multiple $p p$ collisions occurring in the same or neighbouring bunch crossings (pile-up). In the 7 TeV data, the average number of interactions per bunch crossing was approximately 10 ; the average increased to approximately 20 in the 8 TeV data. The reconstruction, identification and isolation criteria used for electrons and photons in the 8 TeV data are improved, making the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$ searches more robust against the increased pile-up. These analyses were re-optimised with simulation and frozen before looking at the 8 TeV data.

In the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channel, the increased pile-up deteriorates the event missing transverse momentum, $E_{\mathrm{T}}^{\text {miss }}$, resolution, which results in significantly larger Drell-Yan background in the same-flavour final states. Since the $e \mu$ channel provides most of the sensitivity of the search, only this final state is used in the analysis of the 8 TeV data. The kinematic region in which a SM Higgs boson with a mass between 110 GeV and 140 GeV is

[^22][^23]searched for was kept blinded during the analysis optimisation, until satisfactory agreement was found between the observed and predicted numbers of events in control samples dominated by the principal backgrounds.

This Letter is organised as follows. The ATLAS detector is briefly described in Section 2. The simulation samples and the signal predictions are presented in Section 3. The analyses of the $H \rightarrow$ $Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow \gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ channels are described in Sections 4-6, respectively. The statistical procedure used to analyse the results is summarised in Section 7. The systematic uncertainties which are correlated between datasets and search channels are described in Section 8. The results of the combination of all channels are reported in Section 9, while Section 10 provides the conclusions.

## 2. The ATLAS detector

The ATLAS detector [19-21] is a multipurpose particle physics apparatus with forward-backward symmetric cylindrical geometry. The inner tracking detector (ID) consists of a silicon pixel detector, a silicon microstrip detector (SCT), and a straw-tube transition radiation tracker (TRT). The ID is surrounded by a thin superconducting solenoid which provides a 2 T magnetic field, and by highgranularity liquid-argon (LAr) sampling electromagnetic calorimetry. The electromagnetic calorimeter is divided into a central barrel (pseudorapidity ${ }^{2}|\eta|<1.475$ ) and end-cap regions on either end of the detector ( $1.375<|\eta|<2.5$ for the outer wheel and $2.5<|\eta|<3.2$ for the inner wheel). In the region matched to the ID $(|\eta|<2.5)$, it is radially segmented into three layers. The first layer has a fine segmentation in $\eta$ to facilitate $e / \gamma$ separation from $\pi^{0}$ and to improve the resolution of the shower position and direction measurements. In the region $|\eta|<1.8$, the electromagnetic calorimeter is preceded by a presampler detector to correct for upstream energy losses. An iron-scintillator/tile calorimeter gives hadronic coverage in the central rapidity range ( $|\eta|<1.7$ ), while a LAr hadronic end-cap calorimeter provides coverage over $1.5<$ $|\eta|<3.2$. The forward regions ( $3.2<|\eta|<4.9$ ) are instrumented with LAr calorimeters for both electromagnetic and hadronic measurements. The muon spectrometer (MS) surrounds the calorimeters and consists of three large air-core superconducting magnets providing a toroidal field, each with eight coils, a system of precision tracking chambers, and fast detectors for triggering. The combination of all these systems provides charged particle measurements together with efficient and precise lepton and photon measurements in the pseudorapidity range $|\eta|<2.5$. Jets and $E_{\mathrm{T}}^{\text {miss }}$ are reconstructed using energy deposits over the full coverage of the calorimeters, $|\eta|<4.9$.

## 3. Signal and background simulation samples

The SM Higgs boson production processes considered in this analysis are the dominant gluon fusion ( $g g \rightarrow H$, denoted ggF ), vector-boson fusion ( $q q^{\prime} \rightarrow q q^{\prime} H$, denoted VBF) and Higgs-strahlung ( $q q^{\prime} \rightarrow W H, Z H$, denoted $W H / Z H$ ). The small contribution from the associated production with a $t \bar{t}$ pair ( $q \bar{q} / g g \rightarrow t \bar{t} H$, denoted $t \bar{t} H$ ) is taken into account only in the $H \rightarrow \gamma \gamma$ analysis.

For the ggF process, the signal cross section is computed at up to next-to-next-to-leading order (NNLO) in QCD [22-28]. Next-to-

[^24]Table 1
Event generators used to model the signal and background processes. "PYTHIA" indicates that PYTHIA6 and PYTHIA8 are used for simulations of $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data, respectively.

| Process | Generator |
| :--- | :--- |
| ggF, VBF | POWHEG [57,58] + PYTHIA |
| $W H, Z H, t \bar{t} H$ | PYTHIA |
| $W+$ jets, $Z / \gamma^{*}+$ jets | ALPGEN [59] + HERWIG |
| $t \bar{t}, t W, t b$ | MC@NLO [60] + HERWIG |
| $t q b$ | AcerMC [61] + PYTHIA |
| $q \bar{q} \rightarrow W W$ | MC@NLO + HERWIG |
| $g g \rightarrow W W$ | gg2WW [62] + HERWIG |
| $q \bar{q} \rightarrow Z Z$ | POWHEG [63] + PYTHIA |
| $g g \rightarrow Z Z$ | gg2ZZ [64] + HERWIG |
| $W Z$ | MadGraph + PYTHIA, HERWIG |
| $W \gamma+$ jets | ALPGEN + HERWIG |
| $W \gamma^{*}[65]$ | MadGraph + PYTHIA |
| $q \bar{q} / g g \rightarrow \gamma \gamma$ | SHERPA |

leading order (NLO) electroweak (EW) corrections are applied [29, 30], as well as QCD soft-gluon re-summations at up to next-to-next-to-leading logarithm (NNLL) [31]. These calculations, which are described in Refs. [32-35], assume factorisation between QCD and EW corrections. The transverse momentum, $p_{\mathrm{T}}$, spectrum of the Higgs boson in the ggF process follows the HqT calculation [36], which includes QCD corrections at NLO and QCD soft-gluon re-summations up to NNLL; the effects of finite quark masses are also taken into account [37].

For the VBF process, full QCD and EW corrections up to NLO [38-41] and approximate NNLO QCD corrections [42] are used to calculate the cross section. Cross sections of the associated $W H / Z H$ processes $(\mathrm{VH})$ are calculated including QCD corrections up to NNLO [43-45] and EW corrections up to NLO [46]. The cross sections for the $t \bar{t} H$ process are estimated up to NLO QCD [47-51].

The total cross sections for SM Higgs boson production at the LHC with $m_{H}=125 \mathrm{GeV}$ are predicted to be 17.5 pb for $\sqrt{s}=$ 7 TeV and 22.3 pb for $\sqrt{s}=8 \mathrm{TeV}[52,53]$.

The branching ratios of the SM Higgs boson as a function of $m_{H}$, as well as their uncertainties, are calculated using the HDECAY [54] and PROPHECY4F [55,56] programs and are taken from Refs. [52,53]. The interference in the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ final states with identical leptons is taken into account [55,56,53].

The event generators used to model signal and background processes in samples of Monte Carlo (MC) simulated events are listed in Table 1. The normalisations of the generated samples are obtained from the state of the art calculations described above. Several different programs are used to generate the hard-scattering processes. To generate parton showers and their hadronisation, and to simulate the underlying event [66-68], PYTHIA6 [69] (for 7 TeV samples and 8 TeV samples produced with MadGraph [70,71] or AcerMC) or PYTHIA8 [72] (for other 8 TeV samples) are used. Alternatively, HERWIG [73] or SHERPA [74] are used to generate and hadronise parton showers, with the HERWIG underlying event simulation performed using JIMMY [75]. When PYTHIA6 or HERWIG are used, TAUOLA [76] and PHOTOS [77] are employed to describe tau lepton decays and additional photon radiation from charged leptons, respectively.

The following parton distribution function (PDF) sets are used: CT10 [78] for the POWHEG, MC@NLO, gg2WW and gg2ZZ samples; CTEQ6L1 [79] for the PYTHIA8, ALPGEN, AcerMC, MadGraph, HERWIG and SHERPA samples; and MRSTMCal [80] for the PYTHIA6 samples.

Acceptances and efficiencies are obtained mostly from full simulations of the ATLAS detector [81] using Geant4 [82]. These simulations include a realistic modelling of the pile-up conditions observed in the data. Corrections obtained from measurements in
data are applied to account for small differences between data and simulation (e.g. large samples of $W, Z$ and $J / \psi$ decays are used to derive scale factors for lepton reconstruction and identification efficiencies).

## 4. $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ channel

The search for the SM Higgs boson through the decay $H \rightarrow$ $Z Z^{(*)} \rightarrow 4 \ell$, where $\ell=e$ or $\mu$, provides good sensitivity over a wide mass range ( $110-600 \mathrm{GeV}$ ), largely due to the excellent momentum resolution of the ATLAS detector. This analysis searches for Higgs boson candidates by selecting two pairs of isolated leptons, each of which is comprised of two leptons with the same flavour and opposite charge. The expected cross section times branching ratio for the process $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ with $m_{H}=125 \mathrm{GeV}$ is 2.2 fb for $\sqrt{s}=7 \mathrm{TeV}$ and 2.8 fb for $\sqrt{s}=8 \mathrm{TeV}$.

The largest background comes from continuum $\left(Z^{(*)} / \gamma^{*}\right)\left(Z^{(*)} /\right.$ $\gamma^{*}$ ) production, referred to hereafter as $Z Z^{(*)}$. For low masses there are also important background contributions from $Z+$ jets and $t \bar{t}$ production, where charged lepton candidates arise either from decays of hadrons with $b$ - or $c$-quark content or from misidentification of jets.

The 7 TeV data have been re-analysed and combined with the 8 TeV data. The analysis is improved in several aspects with respect to Ref. [83] to enhance the sensitivity to a low-mass Higgs boson. In particular, the kinematic selections are revised, and the 8 TeV data analysis benefits from improvements in the electron reconstruction and identification. The expected signal significances for a Higgs boson with $m_{H}=125 \mathrm{GeV}$ are $1.6 \sigma$ for the 7 TeV data (to be compared with $1.25 \sigma$ in Ref. [83]) and $2.1 \sigma$ for the 8 TeV data.

### 4.1. Event selection

The data are selected using single-lepton or dilepton triggers. For the single-muon trigger, the $p_{\mathrm{T}}$ threshold is 18 GeV for the 7 TeV data and 24 GeV for the 8 TeV data, while for the singleelectron trigger the transverse energy, $E_{\mathrm{T}}$, threshold varies from 20 GeV to 22 GeV for the 7 TeV data and is 24 GeV for the 8 TeV data. For the dielectron triggers, the thresholds are 12 GeV for both electrons. For the dimuon triggers, the thresholds for the 7 TeV data are 10 GeV for each muon, while for the 8 TeV data the thresholds are 13 GeV . An additional asymmetric dimuon trigger is used in the 8 TeV data with thresholds 18 GeV and 8 GeV for the leading and sub-leading muon, respectively.

Muon candidates are formed by matching reconstructed ID tracks with either a complete track or a track-segment reconstructed in the MS [84]. The muon acceptance is extended with respect to Ref. [83] using tracks reconstructed in the forward region of the MS $(2.5<|\eta|<2.7)$, which is outside the ID coverage. If both an ID and a complete MS track are present, the two independent momentum measurements are combined; otherwise the information of the ID or the MS is used alone. Electron candidates must have a well-reconstructed ID track pointing to an electromagnetic calorimeter cluster and the cluster should satisfy a set of identification criteria [85] that require the longitudinal and transverse shower profiles to be consistent with those expected for electromagnetic showers. Tracks associated with electromagnetic clusters are fitted using a Gaussian-Sum Filter [86], which allows for bremsstrahlung energy losses to be taken into account.

Each electron (muon) must satisfy $p_{\mathrm{T}}>7 \mathrm{GeV}\left(p_{\mathrm{T}}>6 \mathrm{GeV}\right)$ and be measured in the pseudorapidity range $|\eta|<2.47$ ( $|\eta|<2.7$ ). All possible quadruplet combinations with same-flavour oppositecharge lepton pairs are then formed. The most energetic lepton in the quadruplet must satisfy $p_{\mathrm{T}}>20 \mathrm{GeV}$, and the second (third)
lepton in $p_{\mathrm{T}}$ order must satisfy $p_{\mathrm{T}}>15 \mathrm{GeV}\left(p_{\mathrm{T}}>10 \mathrm{GeV}\right)$. At least one of the leptons must satisfy the single-lepton trigger or one pair must satisfy the dilepton trigger requirements. The leptons are required to be separated from each other by $\Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}>0.1$ if they are of the same flavour and by $\Delta R>0.2$ otherwise. The longitudinal impact parameters of the leptons along the beam axis are required to be within 10 mm of the reconstructed primary vertex. The primary vertex used for the event is defined as the reconstructed vertex with the highest $\sum p_{\mathrm{T}}^{2}$ of associated tracks and is required to have at least three tracks with $p_{\mathrm{T}}>0.4 \mathrm{GeV}$. To reject cosmic rays, muon tracks are required to have a transverse impact parameter, defined as the distance of closest approach to the primary vertex in the transverse plane, of less than 1 mm .

The same-flavour and opposite-charge lepton pair with an invariant mass closest to the $Z$ boson mass ( $m_{Z}$ ) in the quadruplet is referred to as the leading lepton pair. Its invariant mass, denoted by $m_{12}$, is required to be between 50 GeV and 106 GeV . The remaining same-flavour, opposite-charge lepton pair is the subleading lepton pair. Its invariant mass, $m_{34}$, is required to be in the range $m_{\min }<m_{34}<115 \mathrm{GeV}$, where the value of $m_{\min }$ depends on the reconstructed four-lepton invariant mass, $m_{4 \ell}$. The value of $m_{\min }$ varies monotonically from 17.5 GeV at $m_{4 \ell}=120 \mathrm{GeV}$ to 50 GeV at $m_{4 \ell}=190 \mathrm{GeV}$ [87] and is constant above this value. All possible lepton pairs in the quadruplet that have the same flavour and opposite charge must satisfy $m_{\ell \ell}>5 \mathrm{GeV}$ in order to reject backgrounds involving the production and decay of $J / \psi$ mesons. If two or more quadruplets satisfy the above selection, the one with the highest value of $m_{34}$ is selected. Four different analysis sub-channels, $4 e, 2 e 2 \mu, 2 \mu 2 e$ and $4 \mu$, arranged by the flavour of the leading lepton pair, are defined.

Non-prompt leptons from heavy flavour decays, electrons from photon conversions and jets mis-identified as electrons have broader transverse impact parameter distributions than prompt leptons from $Z$ boson decays and/or are non-isolated. Thus, the $Z+$ jets and $t \bar{t}$ background contributions are reduced by applying a cut on the transverse impact parameter significance, defined as the transverse impact parameter divided by its uncertainty, $d_{0} / \sigma_{d_{0}}$. This is required to be less than 3.5 (6.5) for muons (electrons). The electron impact parameter is affected by bremsstrahlung and thus has a broader distribution.

In addition, leptons must satisfy isolation requirements based on tracking and calorimetric information. The normalised track isolation discriminant is defined as the sum of the transverse momenta of tracks inside a cone of size $\Delta R=0.2$ around the lepton direction, excluding the lepton track, divided by the lepton $p_{\mathrm{T}}$. The tracks considered in the sum are those compatible with the lepton vertex and have $p_{\mathrm{T}}>0.4 \mathrm{GeV}\left(p_{\mathrm{T}}>1 \mathrm{GeV}\right)$ in the case of electron (muon) candidates. Each lepton is required to have a normalised track isolation smaller than 0.15 . The normalised calorimetric isolation for electrons is computed as the sum of the $E_{T}$ of positive-energy topological clusters [88] with a reconstructed barycentre falling within a cone of size $\Delta R=0.2$ around the candidate electron cluster, divided by the electron $E_{\mathrm{T}}$. The algorithm for topological clustering suppresses noise by keeping cells with a significant energy deposit and their neighbours. The summed energy of the cells assigned to the electron cluster is excluded, while a correction is applied to account for the electron energy deposited outside the cluster. The ambient energy deposition in the event from pile-up and the underlying event is accounted for using a calculation of the median transverse energy density from low$p_{\mathrm{T}}$ jets [89,90]. The normalised calorimetric isolation for electrons is required to be less than 0.20 . The normalised calorimetric isolation discriminant for muons is defined by the ratio to the $p_{\mathrm{T}}$ of the muon of the $E_{\mathrm{T}}$ sum of the calorimeter cells inside a cone of size
$\Delta R=0.2$ around the muon direction minus the energy deposited by the muon. Muons are required to have a normalised calorimetric isolation less than 0.30 ( 0.15 for muons without an associated ID track). For both the track- and calorimeter-based isolation, any contributions arising from other leptons of the quadruplet are subtracted.

The combined signal reconstruction and selection efficiencies for a SM Higgs with $m_{H}=125 \mathrm{GeV}$ for the $7 \mathrm{TeV}(8 \mathrm{TeV})$ data are $37 \%$ ( $36 \%$ ) for the $4 \mu$ channel, $20 \%$ ( $22 \%$ ) for the $2 e 2 \mu / 2 \mu 2 e$ channels and $15 \%$ ( $20 \%$ ) for the $4 e$ channel.

The $4 \ell$ invariant mass resolution is improved by applying a Z-mass constrained kinematic fit to the leading lepton pair for $m_{4 \ell}<190 \mathrm{GeV}$ and to both lepton pairs for higher masses. The expected width of the reconstructed mass distribution is dominated by the experimental resolution for $m_{H}<350 \mathrm{GeV}$, and by the natural width of the Higgs boson for higher masses ( 30 GeV at $m_{H}=400 \mathrm{GeV}$ ). The typical mass resolutions for $m_{H}=125 \mathrm{GeV}$ are $1.7 \mathrm{GeV}, 1.7 \mathrm{GeV} / 2.2 \mathrm{GeV}$ and 2.3 GeV for the $4 \mu, 2 e 2 \mu / 2 \mu 2 e$ and $4 e$ sub-channels, respectively.

### 4.2. Background estimation

The expected background yield and composition are estimated using the MC simulation normalised to the theoretical cross section for $Z Z^{(*)}$ production and by methods using control regions from data for the $Z+$ jets and $t \bar{t}$ processes. Since the background composition depends on the flavour of the sub-leading lepton pair, different approaches are taken for the $\ell \ell+\mu \mu$ and the $\ell \ell+e e$ final states. The transfer factors needed to extrapolate the background yields from the control regions defined below to the signal region are obtained from the MC simulation. The MC description of the selection efficiencies for the different background components has been verified with data.

The reducible $\ell \ell+\mu \mu$ background is dominated by $t \bar{t}$ and $Z+$ jets (mostly $Z b \bar{b}$ ) events. A control region is defined by removing the isolation requirement on the leptons in the sub-leading pair, and by requiring that at least one of the sub-leading muons fails the transverse impact parameter significance selection. These modifications remove $Z Z^{(*)}$ contributions, and allow both the $t \bar{t}$ and $Z+$ jets backgrounds to be estimated simultaneously using a fit to the $m_{12}$ distribution. The $t \bar{t}$ background contribution is cross-checked by selecting a control sample of events with an opposite charge $e \mu$ pair with an invariant mass between 50 GeV and 106 GeV , accompanied by an opposite-charge muon pair. Events with a $Z$ candidate decaying to a pair of electrons or muons in the aforementioned mass range are excluded. Isolation and transverse impact parameter significance requirements are applied only to the leptons of the $e \mu$ pair.

In order to estimate the reducible $\ell \ell+e e$ background, a control region is formed by relaxing the selection criteria for the electrons of the sub-leading pair. The different sources of electron background are then separated into categories consisting of nonprompt leptons from heavy flavour decays, electrons from photon conversions and jets mis-identified as electrons, using appropriate discriminating variables [91]. This method allows the sum of the $Z+$ jets and $t \bar{t}$ background contributions to be estimated. As a cross-check, the same method is also applied to a similar control region containing same-charge sub-leading electron pairs. An additional cross-check of the $\ell \ell+e e$ background estimation is performed by using a control region with same-charge sub-leading electron pairs, where the three highest $p_{\mathrm{T}}$ leptons satisfy all the analysis criteria whereas the selection cuts are relaxed for the remaining electrons. All the cross-checks yield consistent results.

The data-driven background estimates are summarised in Table 2 . The distribution of $m_{34}$, for events selected by the analysis

Table 2
Summary of the estimated numbers of $Z+$ jets and $t \bar{t}$ background events, for the $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data in the entire phase-space of the analysis after the kinematic selections described in the text. The backgrounds are combined for the $2 \mu 2 e$ and $4 e$ channels, as discussed in the text. The first uncertainty is statistical, while the second is systematic.

| Background | Estimated numbers of events |  |
| :--- | :--- | :--- |
|  | $\sqrt{s}=7 \mathrm{TeV}$ | $\sqrt{s}=8 \mathrm{TeV}$ |
| $4 \mu$ | $0.3 \pm 0.1 \pm 0.1$ | $0.5 \pm 0.1 \pm 0.2$ |
| $Z+$ jets | $0.02 \pm 0.02 \pm 0.01$ | $0.04 \pm 0.02 \pm 0.02$ |
| $t \bar{t}$ |  |  |
| $2 e 2 \mu$ | $0.2 \pm 0.1 \pm 0.1$ | $0.4 \pm 0.1 \pm 0.1$ |
| $Z+$ jets | $0.02 \pm 0.01 \pm 0.01$ | $0.04 \pm 0.01 \pm 0.01$ |
| $t \bar{t}$ |  | $4.9 \pm 0.8 \pm 0.7$ |
| $2 \mu 2 e$ | $2.6 \pm 0.4 \pm 0.4$ |  |
| $Z+$ jets, $t \bar{t}$ | $3.1 \pm 0.6 \pm 0.5$ |  |
| $4 e$ |  | $3.9 \pm 0.7 \pm 0.8$ |
| $Z+$ jets, $t \bar{t}$ |  |  |



Fig. 1. Invariant mass distribution of the sub-leading lepton pair ( $m_{34}$ ) for a sample defined by the presence of a $Z$ boson candidate and an additional same-flavour electron or muon pair, for the combination of $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data in the entire phase-space of the analysis after the kinematic selections described in the text. Isolation and transverse impact parameter significance requirements are applied to the leading lepton pair only. The MC is normalised to the data-driven background estimations. The relatively small contribution of a SM Higgs with $m_{H}=$ 125 GeV in this sample is also shown.
except that the isolation and transverse impact parameter requirements for the sub-leading lepton pair are removed, is presented in Fig. 1.

### 4.3. Systematic uncertainties

The uncertainties on the integrated luminosities are determined to be $1.8 \%$ for the 7 TeV data and $3.6 \%$ for the 8 TeV data using the techniques described in Ref. [92].

The uncertainties on the lepton reconstruction and identification efficiencies and on the momentum scale and resolution are determined using samples of $W, Z$ and $J / \psi$ decays [85, 84]. The relative uncertainty on the signal acceptance due to the uncertainty on the muon reconstruction and identification efficiency is $\pm 0.7 \%$ ( $\pm 0.5 \% / \pm 0.5 \%$ ) for the $4 \mu$ ( $2 e 2 \mu / 2 \mu 2 e$ ) channel for $m_{4 \ell}=600 \mathrm{GeV}$ and increases to $\pm 0.9 \%( \pm 0.8 \% / \pm 0.5 \%)$ for $m_{4 \ell}=115 \mathrm{GeV}$. Similarly, the relative uncertainty on the signal acceptance due to the uncertainty on the electron reconstruction and identification efficiency is $\pm 2.6 \%( \pm 1.7 \% / \pm 1.8 \%)$ for the $4 e(2 e 2 \mu / 2 \mu 2 e)$ channel for $m_{4 \ell}=600 \mathrm{GeV}$ and reaches $\pm 8.0 \%$


Fig. 2. The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates, compared to the background expectation in the $80-250 \mathrm{GeV}$ mass range, for the combination of the $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data. The signal expectation for a SM Higgs with $m_{H}=125 \mathrm{GeV}$ is also shown.

Table 3
The numbers of expected signal ( $m_{H}=125 \mathrm{GeV}$ ) and background events, together with the numbers of observed events in the data, in a window of size $\pm 5 \mathrm{GeV}$ around 125 GeV , for the combined $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data.

|  | Signal | $Z Z^{(*)}$ | $Z+$ jets, $t \bar{t}$ | Observed |
| :--- | :--- | :--- | :--- | :--- |
| $4 \mu$ | $2.09 \pm 0.30$ | $1.12 \pm 0.05$ | $0.13 \pm 0.04$ | 6 |
| $2 e 2 \mu / 2 \mu 2 e$ | $2.29 \pm 0.33$ | $0.80 \pm 0.05$ | $1.27 \pm 0.19$ | 5 |
| $4 e$ | $0.90 \pm 0.14$ | $0.44 \pm 0.04$ | $1.09 \pm 0.20$ | 2 |

$( \pm 2.3 \% / \pm 7.6 \%)$ for $m_{4 \ell}=115 \mathrm{GeV}$. The uncertainty on the electron energy scale results in an uncertainty of $\pm 0.7 \%( \pm 0.5 \% / \pm 0.2 \%)$ on the mass scale of the $m_{4 \ell}$ distribution for the $4 e(2 e 2 \mu / 2 \mu 2 e)$ channel. The impact of the uncertainties on the electron energy resolution and on the muon momentum resolution and scale are found to be negligible.

The theoretical uncertainties associated with the signal are described in detail in Section 8. For the SM $Z Z^{(*)}$ background, which is estimated from MC simulation, the uncertainty on the total yield due to the QCD scale uncertainty is $\pm 5 \%$, while the effect of the PDF and $\alpha_{s}$ uncertainties is $\pm 4 \%( \pm 8 \%)$ for processes initiated by quarks (gluons) [53]. In addition, the dependence of these uncertainties on the four-lepton invariant mass spectrum has been taken into account as discussed in Ref. [53]. Though a small excess of events is observed for $m_{4 l}>160 \mathrm{GeV}$, the measured $Z Z^{(*)} \rightarrow 4 \ell$ cross section [93] is consistent with the SM theoretical prediction. The impact of not using the theoretical constraints on the $Z Z^{(*)}$ yield on the search for a Higgs boson with $m_{H}<2 m_{Z}$ has been studied in Ref. [87] and has been found to be negligible. The impact of the interference between a Higgs signal and the nonresonant $g g \rightarrow Z Z^{(*)}$ background is small and becomes negligible for $m_{H}<2 m_{Z}$ [94].

### 4.4. Results

The expected distributions of $m_{4 \ell}$ for the background and for a Higgs boson signal with $m_{H}=125 \mathrm{GeV}$ are compared to the data in Fig. 2. The numbers of observed and expected events in a window of $\pm 5 \mathrm{GeV}$ around $m_{H}=125 \mathrm{GeV}$ are presented for the combined 7 TeV and 8 TeV data in Table 3. The distribution of the $m_{34}$ versus $m_{12}$ invariant mass is shown in Fig. 3. The statistical interpretation of the excess of events near $m_{4 \ell}=125 \mathrm{GeV}$ in Fig. 2 is presented in Section 9.


Fig. 3. Distribution of the $m_{34}$ versus the $m_{12}$ invariant mass, before the application of the $Z$-mass constrained kinematic fit, for the selected candidates in the $m_{4 \ell}$ range $120-130 \mathrm{GeV}$. The expected distributions for a SM Higgs with $m_{H}=125 \mathrm{GeV}$ (the sizes of the boxes indicate the relative density) and for the total background (the intensity of the shading indicates the relative density) are also shown.

## 5. $H \rightarrow \gamma \gamma$ channel

The search for the SM Higgs boson through the decay $H \rightarrow \gamma \gamma$ is performed in the mass range between 110 GeV and 150 GeV . The dominant background is SM diphoton production $(\gamma \gamma)$; contributions also come from $\gamma+$ jet and jet + jet production with one or two jets mis-identified as photons ( $\gamma j$ and $j j$ ) and from the Drell-Yan process. The 7 TeV data have been re-analysed and the results combined with those from the 8 TeV data. Among other changes to the analysis, a new category of events with two jets is introduced, which enhances the sensitivity to the VBF process. Higgs boson events produced by the VBF process have two forward jets, originating from the two scattered quarks, and tend to be devoid of jets in the central region. Overall, the sensitivity of the analysis has been improved by about $20 \%$ with respect to that described in Ref. [95].

### 5.1. Event selection

The data used in this channel are selected using a diphoton trigger [96], which requires two clusters formed from energy depositions in the electromagnetic calorimeter. An $E_{\mathrm{T}}$ threshold of 20 GeV is applied to each cluster for the 7 TeV data, while for the 8 TeV data the thresholds are increased to 35 GeV on the leading (the highest $E_{\mathrm{T}}$ ) cluster and to 25 GeV on the sub-leading (the next-highest $E_{T}$ ) cluster. In addition, loose criteria are applied to the shapes of the clusters to match the expectations for electromagnetic showers initiated by photons. The efficiency of the trigger is greater than $99 \%$ for events passing the final event selection.

Events are required to contain at least one reconstructed vertex with at least two associated tracks with $p_{\mathrm{T}}>0.4 \mathrm{GeV}$, as well as two photon candidates. Photon candidates are reconstructed in the fiducial region $|\eta|<2.37$, excluding the calorimeter barrel/endcap transition region $1.37 \leqslant|\eta|<1.52$. Photons that convert to electron-positron pairs in the ID material can have one or two reconstructed tracks matched to the clusters in the calorimeter. The photon reconstruction efficiency is about $97 \%$ for $E_{\mathrm{T}}>30 \mathrm{GeV}$.

In order to account for energy losses upstream of the calorimeter and energy leakage outside of the cluster, MC simulation results are used to calibrate the energies of the photon candidates; there are separate calibrations for unconverted and converted
candidates. The calibration is refined by applying $\eta$-dependent correction factors, which are of the order of $\pm 1 \%$, determined from measured $Z \rightarrow e^{+} e^{-}$events. The leading (sub-leading) photon candidate is required to have $E_{\mathrm{T}}>40 \mathrm{GeV}(30 \mathrm{GeV})$.

Photon candidates are required to pass identification criteria based on shower shapes in the electromagnetic calorimeter and on energy leakage into the hadronic calorimeter [97]. For the 7 TeV data, this information is combined in a neural network, tuned to achieve a similar jet rejection as the cut-based selection described in Ref. [95], but with higher photon efficiency. For the 8 TeV data, cut-based criteria are used to ensure reliable photon performance for recently-recorded data. This cut-based selection has been tuned to be robust against pile-up by relaxing requirements on shower shape criteria more susceptible to pile-up, and tightening others. The photon identification efficiencies, averaged over $\eta$, range from $85 \%$ to above $95 \%$ for the $E_{\mathrm{T}}$ range under consideration.

To further suppress the jet background, an isolation requirement is applied. The isolation transverse energy is defined as the sum of the transverse energy of positive-energy topological clusters, as described in Section 4, within a cone of size $\Delta R=0.4$ around the photon candidate, excluding the region within $0.125 \times$ 0.175 in $\Delta \eta \times \Delta \phi$ around the photon barycentre. The distributions of the isolation transverse energy in data and simulation have been found to be in good agreement using electrons from $Z \rightarrow e^{+} e^{-}$ events and photons from $Z \rightarrow \ell^{+} \ell^{-} \gamma$ events. Remaining small differences are taken into account as a systematic uncertainty. Photon candidates are required to have an isolation transverse energy of less than 4 GeV .

### 5.2. Invariant mass reconstruction

The invariant mass of the two photons is evaluated using the photon energies measured in the calorimeter, the azimuthal angle $\phi$ between the photons as determined from the positions of the photons in the calorimeter, and the values of $\eta$ calculated from the position of the identified primary vertex and the impact points of the photons in the calorimeter.

The primary vertex of the hard interaction is identified by combining the following information in a global likelihood: the directions of flight of the photons as determined using the longitudinal segmentation of the electromagnetic calorimeter (calorimeter pointing), the parameters of the beam spot, and the $\sum p_{\mathrm{T}}^{2}$ of the tracks associated with each reconstructed vertex. In addition, for the 7 TeV data analysis, the reconstructed conversion vertex is used in the likelihood for converted photons with tracks containing hits in the silicon layers of the ID. The calorimeter pointing is sufficient to ensure that the contribution of the opening angle between the photons to the mass resolution is negligible. Using the calorimeter pointing alone, the resolution of the vertex $z$ coordinate is $\sim 15 \mathrm{~mm}$, improving to $\sim 6 \mathrm{~mm}$ for events with two reconstructed converted photons. The tracking information from the ID improves the identification of the vertex of the hard interaction, which is needed for the jet selection in the 2-jet category.

With the selection described in Section 5.1, in the diphoton invariant mass range between 100 GeV and $160 \mathrm{GeV}, 23788$ and 35251 diphoton candidates are observed in the 7 TeV and 8 TeV data samples, respectively.

Data-driven techniques [98] are used to estimate the numbers of $\gamma \gamma, \gamma j$ and $j j$ events in the selected sample. The contribution from the Drell-Yan background is determined from a sample of $Z \rightarrow e^{+} e^{-}$decays in data where either one or both electrons pass the photon selection. The measured composition of the selected sample is approximately $74 \%, 22 \%, 3 \%$ and $1 \%$ for the $\gamma \gamma, \gamma j$, $j j$ and Drell-Yan processes, respectively, demonstrating the dominance of the irreducible diphoton production. This decomposition
is not directly used in the signal search; however, it is used to study the parameterisation of the background modelling.

### 5.3. Event categorisation

To increase the sensitivity to a Higgs boson signal, the events are separated into ten mutually exclusive categories having different mass resolutions and signal-to-background ratios. An exclusive category of events containing two jets improves the sensitivity to VBF. The other nine categories are defined by the presence or not of converted photons, $\eta$ of the selected photons, and $p_{\mathrm{Tt}}$, the component ${ }^{3}$ of the diphoton $p_{\mathrm{T}}$ that is orthogonal to the axis defined by the difference between the two photon momenta [99,100].

Jets are reconstructed [101] using the anti- $k_{t}$ algorithm [102] with radius parameter $R=0.4$. At least two jets with $|\eta|<4.5$ and $p_{\mathrm{T}}>25 \mathrm{GeV}$ are required in the 2 -jet selection. In the analysis of the 8 TeV data, the $p_{\mathrm{T}}$ threshold is raised to 30 GeV for jets with $2.5<|\eta|<4.5$. For jets in the ID acceptance ( $|\eta|<2.5$ ), the fraction of the sum of the $p_{\mathrm{T}}$ of tracks, associated with the jet and matched to the selected primary vertex, with respect to the sum of the $p_{\text {T }}$ of tracks associated with the jet (jet vertex fraction, JVF) is required to be at least 0.75 . This requirement on the JVF reduces the number of jets from proton-proton interactions not associated with the primary vertex. Motivated by the VBF topology, three additional cuts are applied in the 2-jet selection: the difference of the pseudorapidity between the leading and sub-leading jets (tag jets) is required to be larger than 2.8 , the invariant mass of the tag jets has to be larger than 400 GeV , and the azimuthal angle difference between the diphoton system and the system of the tag jets has to be larger than 2.6 . About $70 \%$ of the signal events in the 2-jet category come from the VBF process.

The other nine categories are defined as follows: events with two unconverted photons are separated into unconverted central ( $|\eta|<0.75$ for both candidates) and unconverted rest (all other events), events with at least one converted photon are separated into converted central ( $|\eta|<0.75$ for both candidates), converted transition (at least one photon with $1.3<|\eta|<1.75$ ) and converted rest (all other events). Except for the converted transition category, each category is further divided by a cut at $p_{\mathrm{Tt}}=60 \mathrm{GeV}$ into two categories, low $p_{\text {Tt }}$ and high $p_{\text {Tt }}$. MC studies show that signal events, particularly those produced via VBF or associated production ( $W H / Z H$ and $t \bar{t} H$ ), have on average larger $p_{\mathrm{Tt}}$ than background events. The number of data events in each category, as well as the sum of all the categories, which is denoted inclusive, are given in Table 4.

### 5.4. Signal modelling

The description of the Higgs boson signal is obtained from MC, as described in Section 3. The cross sections multiplied by the branching ratio into two photons are given in Table 4 for $m_{H}=126.5 \mathrm{GeV}$. The number of signal events produced via the ggF process is rescaled to take into account the expected destructive interference between the $g g \rightarrow \gamma \gamma$ continuum background and $\operatorname{ggF}$ [103], leading to a reduction of the production rate by $2-5 \%$ depending on $m_{H}$ and the event category. For both the 7 TeV and 8 TeV MC samples, the fractions of ggF, VBF, $W H, Z H$ and $t \bar{t} H$ production are approximately $88 \%, 7 \%, 3 \%, 2 \%$ and $0.5 \%$, respectively, for $m_{H}=126.5 \mathrm{GeV}$.

In the simulation, the shower shape distributions are shifted slightly to improve the agreement with the data [97], and the

[^25]Table 4
Number of events in the data ( $N_{\mathrm{D}}$ ) and expected number of signal events ( $N_{\mathrm{S}}$ ) for $m_{H}=126.5 \mathrm{GeV}$ from the $H \rightarrow \gamma \gamma$ analysis, for each category in the mass range $100-160 \mathrm{GeV}$. The mass resolution FWHM (see text) is also given for the 8 TeV data. The Higgs boson production cross section multiplied by the branching ratio into two photons $(\sigma \times B(H \rightarrow \gamma \gamma))$ is listed for $m_{H}=126.5 \mathrm{GeV}$. The statistical uncertainties on $N_{\mathrm{S}}$ and FWHM are less than $1 \%$.

| $\sqrt{s}$ | 7 TeV |  | 8 TeV |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\sigma \times B(H \rightarrow \gamma \gamma)[\mathrm{fb}]$ | 39 |  | 50 |  | FWHM [GeV] |
| Category | $N_{\text {D }}$ | $N_{\text {S }}$ | $N_{\text {D }}$ | $N_{\text {S }}$ |  |
| Unconv. central, low $p_{\text {Tt }}$ | 2054 | 10.5 | 2945 | 14.2 | 3.4 |
| Unconv. central, high $p_{\mathrm{Tt}}$ | 97 | 1.5 | 173 | 2.5 | 3.2 |
| Unconv. rest, low $p_{\text {Tt }}$ | 7129 | 21.6 | 12136 | 30.9 | 3.7 |
| Unconv. rest, high $p_{\text {Tt }}$ | 444 | 2.8 | 785 | 5.2 | 3.6 |
| Conv. central, low $p_{\text {Tt }}$ | 1493 | 6.7 | 2015 | 8.9 | 3.9 |
| Conv. central, high $p_{\text {Tt }}$ | 77 | 1.0 | 113 | 1.6 | 3.5 |
| Conv. rest, low $p_{\text {Tt }}$ | 8313 | 21.1 | 11099 | 26.9 | 4.5 |
| Conv. rest, high $p_{\text {Tt }}$ | 501 | 2.7 | 706 | 4.5 | 3.9 |
| Conv. transition | 3591 | 9.5 | 5140 | 12.8 | 6.1 |
| 2-jet | 89 | 2.2 | 139 | 3.0 | 3.7 |
| All categories (inclusive) | 23788 | 79.6 | 35251 | 110.5 | 3.9 |

photon energy resolution is broadened (by approximately $1 \%$ in the barrel calorimeter and $1.2-2.1 \%$ in the end-cap regions) to account for small differences observed between $Z \rightarrow e^{+} e^{-}$data and MC events. The signal yields expected for the 7 TeV and 8 TeV data samples are given in Table 4. The overall selection efficiency is about $40 \%$.

The shape of the invariant mass of the signal in each category is modelled by the sum of a Crystal Ball function [104], describing the core of the distribution with a width $\sigma_{C B}$, and a Gaussian contribution describing the tails (amounting to $<10 \%$ ) of the mass distribution. The expected full-width-at-half-maximum (FWHM) is 3.9 GeV and $\sigma_{C B}$ is 1.6 GeV for the inclusive sample. The resolution varies with event category (see Table 4); the FWHM is typically a factor 2.3 larger than $\sigma_{C B}$.

### 5.5. Background modelling

The background in each category is estimated from data by fitting the diphoton mass spectrum in the mass range $100-160 \mathrm{GeV}$ with a selected model with free parameters of shape and normalisation. Different models are chosen for the different categories to achieve a good compromise between limiting the size of a potential bias while retaining good statistical power. A fourth-order Bernstein polynomial function [105] is used for the unconverted rest (low $p_{\mathrm{Tt}}$ ), converted rest (low $p_{\mathrm{Tt}}$ ) and inclusive categories, an exponential function of a second-order polynomial for the unconverted central (low $p_{\mathrm{Tt}}$ ), converted central (low $p_{\mathrm{Tt}}$ ) and converted transition categories, and an exponential function for all others.

Studies to determine the potential bias have been performed using large samples of simulated background events complemented by data-driven estimates. The background shapes in the simulation have been cross-checked using data from control regions. The potential bias for a given model is estimated, separately for each category, by performing a maximum likelihood fit to large samples of simulated background events in the mass range 100160 GeV , of the sum of a signal plus the given background model. The signal shape is taken to follow the expectation for a SM Higgs boson; the signal yield is a free parameter of the fit. The potential bias is defined by the largest absolute signal yield obtained from the likelihood fit to the simulated background samples for hypothesised Higgs boson masses in the range $110-150 \mathrm{GeV}$. A pre-selection of background parameterisations is made by requiring that the potential bias, as defined above, is less than $20 \%$ of the statistical uncertainty on the fitted signal yield. The pre-
selected parameterisation in each category with the best expected sensitivity for $m_{H}=125 \mathrm{GeV}$ is selected as the background model.

The largest absolute signal yield as defined above is taken as the systematic uncertainty on the background model. It amounts to $\pm(0.2-4.6)$ and $\pm(0.3-6.8)$ events, depending on the category for the 7 TeV and 8 TeV data samples, respectively. In the final fit to the data (see Section 5.7) a signal-like term is included in the likelihood function for each category. This term incorporates the estimated potential bias, thus providing a conservative estimate of the uncertainty due to the background modelling.

### 5.6. Systematic uncertainties

Hereafter, in cases where two uncertainties are quoted, they refer to the 7 TeV and 8 TeV data, respectively. The dominant experimental uncertainty on the signal yield ( $\pm 8 \%, \pm 11 \%$ ) comes from the photon reconstruction and identification efficiency, which is estimated with data using electrons from $Z$ decays and photons from $Z \rightarrow \ell^{+} \ell^{-} \gamma$ events. Pile-up modelling also affects the expected yields and contributes to the uncertainty ( $\pm 4 \%$ ). Further uncertainties on the signal yield are related to the trigger $( \pm 1 \%)$, photon isolation ( $\pm 0.4 \%, \pm 0.5 \%$ ) and luminosity ( $\pm 1.8 \%, \pm 3.6 \%$ ). Uncertainties due to the modelling of the underlying event are $\pm 6 \%$ for VBF and $\pm 30 \%$ for other production processes in the 2-jet category. Uncertainties on the predicted cross sections and branching ratio are summarised in Section 8.

The uncertainty on the expected fractions of signal events in each category is described in the following. The uncertainty on the knowledge of the material in front of the calorimeter is used to derive the amount of possible event migration between the converted and unconverted categories ( $\pm 4 \%$ ). The uncertainty from pile-up on the population of the converted and unconverted categories is $\pm 2 \%$. The uncertainty from the jet energy scale (JES) amounts to up to $\pm 19 \%$ for the 2-jet category, and up to $\pm 4 \%$ for the other categories. Uncertainties from the JVF modelling are $\pm 12 \%$ (for the 8 TeV data) for the 2-jet category, estimated from $Z+2$-jets events by comparing data and MC. Different PDFs and scale variations in the HqT calculations are used to derive possible event migration among categories $( \pm 9 \%)$ due to the modelling of the Higgs boson kinematics.

The total uncertainty on the mass resolution is $\pm 14 \%$. The dominant contribution ( $\pm 12 \%$ ) comes from the uncertainty on the energy resolution of the calorimeter, which is determined from $Z \rightarrow e^{+} e^{-}$events. Smaller contributions come from the imperfect knowledge of the material in front of the calorimeter, which affects the extrapolation of the calibration from electrons to photons ( $\pm 6 \%$ ), and from pile-up ( $\pm 4 \%$ ).

### 5.7. Results

The distributions of the invariant mass, $m_{\gamma \gamma}$, of the diphoton events, summed over all categories, are shown in Fig. 4(a) and (b). The result of a fit including a signal component fixed to $m_{H}=$ 126.5 GeV and a background component described by a fourthorder Bernstein polynomial is superimposed.

The statistical analysis of the data employs an unbinned likelihood function constructed from those of the ten categories of the 7 TeV and 8 TeV data samples. To demonstrate the sensitivity of this likelihood analysis, Figs. 4(c) and (d) also show the mass spectrum obtained after weighting events with categorydependent factors reflecting the signal-to-background ratios. The weight $w_{i}$ for events in category $i \in[1,10]$ for the 7 TeV and 8 TeV data samples is defined to be $\ln \left(1+S_{i} / B_{i}\right)$, where $S_{i}$ is $90 \%$ of the expected signal for $m_{H}=126.5 \mathrm{GeV}$, and $B_{i}$ is the integral, in


Fig. 4. The distributions of the invariant mass of diphoton candidates after all selections for the combined 7 TeV and 8 TeV data sample. The inclusive sample is shown in (a) and a weighted version of the same sample in (c); the weights are explained in the text. The result of a fit to the data of the sum of a signal component fixed to $m_{H}=126.5 \mathrm{GeV}$ and a background component described by a fourth-order Bernstein polynomial is superimposed. The residuals of the data and weighted data with respect to the respective fitted background component are displayed in (b) and (d).
a window containing $S_{i}$, of a background-only fit to the data. The values $S_{i} / B_{i}$ have only a mild dependence on $m_{H}$.

The statistical interpretation of the excess of events near $m_{\gamma \gamma}=$ 126.5 GeV in Fig. 4 is presented in Section 9.

## 6. $H \rightarrow W W^{(*)} \rightarrow e v \mu \nu$ channel

The signature for this channel is two opposite-charge leptons with large transverse momentum and a large momentum imbalance in the event due to the escaping neutrinos. The dominant backgrounds are non-resonant $W W, t \bar{t}$, and $W t$ production, all of which have real $W$ pairs in the final state. Other important backgrounds include Drell-Yan events ( $p p \rightarrow Z / \gamma^{(*)} \rightarrow \ell \ell$ ) with $E_{\mathrm{T}}^{\text {miss }}$ that may arise from mismeasurement, $W+$ jets events in which a jet produces an object reconstructed as the second electron or muon, and $W \gamma$ events in which the photon undergoes a conversion. Boson pair production ( $W \gamma^{*} / W Z^{(*)}$ and $Z Z^{(*)}$ ) can also produce opposite-charge lepton pairs with additional leptons that are not detected.

The analysis of the 8 TeV data presented here is focused on the mass range $110<m_{H}<200 \mathrm{GeV}$. It follows the procedure used for the 7 TeV data, described in Ref. [106], except that more stringent criteria are applied to reduce the $W+$ jets background and some selections have been modified to mitigate the impact of the higher instantaneous luminosity at the LHC in 2012. In particular, the higher luminosity results in a larger Drell-Yan background to the same-flavour final states, due to the deterioration of the missing transverse momentum resolution. For this reason, and the fact that the $e \mu$ final state provides more than $85 \%$ of the sensitivity of
the search, the same-flavour final states have not been used in the analysis described here.

### 6.1. Event selection

For the $8 \mathrm{TeV} H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ search, the data are selected using inclusive single-muon and single-electron triggers. Both triggers require an isolated lepton with $p_{\mathrm{T}}>24 \mathrm{GeV}$. Quality criteria are applied to suppress non-collision backgrounds such as cosmic-ray muons, beam-related backgrounds, and noise in the calorimeters. The primary vertex selection follows that described in Section 4. Candidates for the $H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ search are pre-selected by requiring exactly two opposite-charge leptons of different flavours, with $p_{\mathrm{T}}$ thresholds of 25 GeV for the leading lepton and 15 GeV for the sub-leading lepton. Events are classified into two exclusive lepton channels depending on the flavour of the leading lepton, where $e \mu(\mu e)$ refers to events with a leading electron (muon). The dilepton invariant mass is required to be greater than 10 GeV .

The lepton selection and isolation have more stringent requirements than those used for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ analysis (see Section 4), to reduce the larger background from non-prompt leptons in the $\ell \nu \ell \nu$ final state. Electron candidates are selected using a combination of tracking and calorimetric information [85]; the criteria are optimised for background rejection, at the expense of some reduced efficiency. Muon candidates are restricted to those with matching MS and ID tracks [84], and therefore are reconstructed over $|\eta|<2.5$. The isolation criteria require the scalar sums of the $p_{\mathrm{T}}$ of charged particles and of calorimeter topological clusters within $\Delta R=0.3$ of the lepton direction (excluding the lepton itself) each to be less than $0.12-0.20$ times the lepton $p_{\mathrm{T}}$. The exact value differs between the criteria for tracks and calorimeter clusters, for both electrons and muons, and depends on the lepton $p_{\mathrm{T}}$. Jet selections follow those described in Section 5.3, except that the JVF is required to be greater than 0.5 .

Since two neutrinos are present in the signal final state, events are required to have large $E_{\mathrm{T}}^{\text {miss }}$. $\mathbf{E}_{\mathrm{T}}^{\text {miss }}$ is the negative vector sum of the transverse momenta of the reconstructed objects, including muons, electrons, photons, jets, and clusters of calorimeter cells not associated with these objects. The quantity $E_{T, \text { rel }}^{\text {miss }}$ used in this analysis is required to be greater than 25 GeV and is defined as: $E_{\mathrm{T}, \text { rel }}^{\text {miss }}=E_{\mathrm{T}}^{\mathrm{miss}} \sin \Delta \phi_{\min }$, where $\Delta \phi_{\min }$ is $\min \left(\Delta \phi, \frac{\pi}{2}\right)$, and $E_{\mathrm{T}}^{\text {miss }}$ is the magnitude of the vector $\mathbf{E}_{\mathrm{T}}^{\text {miss }}$. Here, $\Delta \phi$ is the angle between $\mathbf{E}_{\mathrm{T}}^{\text {miss }}$ and the transverse momentum of the nearest lepton or jet with $p_{\mathrm{T}}>25 \mathrm{GeV}$. Compared to $E_{\mathrm{T}}^{\text {miss }}, E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ has increased rejection power for events in which the $E_{\mathrm{T}}^{\text {miss }}$ is generated by a neutrino in a jet or the mismeasurement of an object, since in those events the $\mathbf{E}_{\mathrm{T}}^{\text {miss }}$ tends to point in the direction of the object. After the lepton isolation and $E_{\mathrm{T}, \mathrm{rel}}^{\text {miss }}$ requirements that define the pre-selected sample, the multijet background is negligible and the Drell-Yan background is much reduced. The Drell-Yan contribution becomes very small after the topological selections, described below, are applied.

The background rate and composition depend significantly on the jet multiplicity, as does the signal topology. Without accompanying jets, the signal originates almost entirely from the ggF process and the background is dominated by $W W$ events. In contrast, when produced in association with two or more jets, the signal contains a much larger contribution from the VBF process compared to the ggF process, and the background is dominated by $t \bar{t}$ production. Therefore, to maximise the sensitivity to SM Higgs events, further selection criteria depending on the jet multiplicity are applied to the pre-selected sample. The data are subdivided into 0 -jet, 1 -jet and 2 -jet search channels according to the number
of jets in the final state, with the 2-jet channel also including higher jet multiplicities.

Owing to spin correlations in the $W W^{(*)}$ system arising from the spin-0 nature of the SM Higgs boson and the V-A structure of the $W$ boson decay vertex, the charged leptons tend to emerge from the primary vertex pointing in the same direction [107]. This kinematic feature is exploited for all jet multiplicities by requiring that $\left|\Delta \phi_{\ell \ell}\right|<1.8$, and the dilepton invariant mass, $m_{\ell \ell}$, be less than 50 GeV for the 0 -jet and 1 -jet channels. For the 2 -jet channel, the $m_{\ell \ell}$ upper bound is increased to 80 GeV .

In the 0 -jet channel, the magnitude $p_{\mathrm{T}}^{\ell \ell}$ of the transverse momentum of the dilepton system, $\mathbf{p}_{\mathrm{T}}^{\ell \ell}=\mathbf{p}_{\mathrm{T}}^{\ell 1}+\mathbf{p}_{\mathrm{T}}^{\ell 2}$, is required to be greater than 30 GeV . This improves the rejection of the Drell-Yan background.

In the 1-jet channel, backgrounds from top quark production are suppressed by rejecting events containing a $b$-tagged jet, as determined using a $b$-tagging algorithm that uses a neural network and exploits the topology of weak decays of $b$ - and $c$-hadrons [108]. The total transverse momentum, $p_{\mathrm{T}}^{\text {tot }}$, defined as the magnitude of the vector sum $\mathbf{p}_{\mathrm{T}}^{\text {tot }}=\mathbf{p}_{\mathrm{T}}^{\ell 1}+\mathbf{p}_{\mathrm{T}}^{\ell 2}+\mathbf{p}_{\mathrm{T}}^{j}+\mathbf{E}_{\mathrm{T}}^{\text {miss }}$, is required to be smaller than 30 GeV to suppress top background events that have jets with $p_{\mathrm{T}}$ below the threshold defined for jet counting. In order to reject the background from $Z \rightarrow \tau \tau$, the $\tau \tau$ invariant mass, $m_{\tau \tau}$, is computed under the assumptions that the reconstructed leptons are $\tau$ lepton decay products. In addition the neutrinos produced in these decays are assumed to be the only source of $E_{\mathrm{T}}^{\text {miss }}$ and to be collinear with the leptons [109]. Events with $\left|m_{\tau \tau}-m_{Z}\right|<25 \mathrm{GeV}$ are rejected if the collinear approximation yields a physical solution.

The 2 -jet selection follows the 1 -jet selection described above, with the $p_{\mathrm{T}}^{\text {tot }}$ definition modified to include all selected jets. Motivated by the VBF topology, several additional criteria are applied to the tag jets, defined as the two highest $-p_{\mathrm{T}}$ jets in the event. These are required to be separated in rapidity by a distance $\left|\Delta y_{j j}\right|>3.8$ and to have an invariant mass, $m_{j j}$, larger than 500 GeV . Events with an additional jet with $p_{\mathrm{T}}>20 \mathrm{GeV}$ between the tag jets ( $y_{j 1}<y<y_{j 2}$ ) are rejected.

A transverse mass variable, $m_{\mathrm{T}}$ [110], is used to test for the presence of a signal for all jet multiplicities. This variable is defined as:
$m_{\mathrm{T}}=\sqrt{\left(E_{\mathrm{T}}^{\ell \ell}+E_{\mathrm{T}}^{\text {miss }}\right)^{2}-\left|\mathbf{p}_{\mathrm{T}}^{\ell \ell}+\mathbf{E}_{\mathrm{T}}^{\text {miss }}\right|^{2}}$,
where $E_{\mathrm{T}}^{\ell \ell}=\sqrt{\left|\mathbf{p}_{\mathrm{T}}^{\ell \ell}\right|^{2}+m_{\ell \ell}^{2}}$. The statistical analysis of the data uses a fit to the $m_{\mathrm{T}}$ distribution in the signal region after the $\Delta \phi_{\ell \ell}$ requirement (see Section 6.4), which results in increased sensitivity compared to the analysis described in Ref. [111].

For a SM Higgs boson with $m_{H}=125 \mathrm{GeV}$, the cross section times branching ratio to the $e \nu \mu \nu$ final state is 88 fb for $\sqrt{s}=7 \mathrm{TeV}$, increasing to 112 fb at $\sqrt{s}=8 \mathrm{TeV}$. The combined acceptance times efficiency of the 8 TeV 0 -jet and 1 -jet selection relative to the ggF production cross section times branching ratio is about $7.4 \%$. The acceptance times efficiency of the 8 TeV 2-jet selection relative to the VBF production cross section times branching ratio is about $14 \%$. Both of these figures are based on the number of events selected before the final $m_{\mathrm{T}}$ criterion is applied (as described in Section 6.4).

### 6.2. Background normalisation and control samples

The leading backgrounds from SM processes producing two isolated high- $p_{\mathrm{T}}$ leptons are $W W$ and top (in this section, "top" background always includes both $t \bar{t}$ and single top, unless otherwise noted). These are estimated using partially data-driven techniques
based on normalising the MC predictions to the data in control regions dominated by the relevant background source. The $W+$ jets background is estimated from data for all jet multiplicities. Only the small backgrounds from Drell-Yan and diboson processes other than $W W$, as well as the $W W$ background for the 2-jet analysis, are estimated using MC simulation.

The control and validation regions are defined by selections similar to those used for the signal region but with some criteria reversed or modified to obtain signal-depleted samples enriched in a particular background. The term "validation region" distinguishes these regions from the control regions that are used to directly normalise the backgrounds. Some control regions have significant contributions from backgrounds other than the targeted one, which introduces dependencies among the background estimates. These correlations are fully incorporated in the fit to the $m_{\mathrm{T}}$ distribution. In the following sections, each background estimate is described after any others on which it depends. Hence, the largest background $(W W)$ is described last.

### 6.2.1. $W+$ jets background estimation

The $W+$ jets background contribution is estimated using a control sample of events where one of the two leptons satisfies the identification and isolation criteria described in Section 6.1, and the other lepton fails these criteria but satisfies a loosened selection (denoted "anti-identified"). Otherwise, events in this sample are required to pass all the signal selections. The dominant contribution to this sample comes from $W+$ jets events in which a jet produces an object that is reconstructed as a lepton. This object may be either a true electron or muon from the decay of a heavy quark, or else a product of the fragmentation identified as a lepton candidate.

The contamination in the signal region is obtained by scaling the number of events in the data control sample by a transfer factor. The transfer factor is defined here as the ratio of the number of identified lepton candidates passing all selections to the number of anti-identified leptons. It is calculated as a function of the anti-identified lepton $p_{\text {T }}$ using a data sample dominated by QCD jet production (dijet sample) after subtracting the residual contributions from leptons produced by leptonic $W$ and $Z$ decays, as estimated from data. The small remaining lepton contamination, which includes $W \gamma^{(*)} / W Z^{(*)}$ events, is subtracted using MC simulation.

The processes producing the majority of same-charge dilepton events, $W+$ jets, $W \gamma^{(*)} / W Z^{(*)}$ and $Z^{(*)} Z^{(*)}$, are all backgrounds in the opposite-charge signal region. $W+$ jets and $W \gamma^{(*)}$ backgrounds are particularly important in a search optimised for a low Higgs boson mass hypothesis. Therefore, the normalisation and kinematic features of same-charge dilepton events are used to validate the predictions of these backgrounds. The predicted number of same-charge events after the $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ and zero-jet requirements is $216 \pm 7$ (stat) $\pm 42$ (syst), while 182 events are observed in the data. Satisfactory agreement between data and simulation is observed in various kinematic distributions, including those of $\Delta \phi_{\ell \ell}$ (see Fig. 5(a)) and the transverse mass.

### 6.2.2. Top control sample

In the 0 -jet channel, the top quark background prediction is first normalised using events satisfying the pre-selection criteria described in Section 6.1. This sample is selected without jet multiplicity or $b$-tagging requirements, and the majority of events contain top quarks. Non-top contributions are subtracted using predictions from simulation, except for $W+$ jets, which is estimated using data. After this normalisation is performed, the fraction of events with zero jets that pass all selections is evaluated. This fraction is small (about 3\%), since the top quark decay $t \rightarrow W b$


Fig. 5. Validation and control distributions for the $H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ analysis. (a) $\Delta \phi_{\ell \ell}$ distribution in the same-charge validation region after the $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ and zerojet requirements. (b) $m_{\mathrm{T}}$ distribution in the $W W$ control region for the 0 -jet channel. The $e \mu$ and $\mu e$ final states are combined. The hashed area indicates the total uncertainty on the background prediction. The expected signal for $m_{H}=125 \mathrm{GeV}$ is negligible and therefore not visible.
has a branching ratio of nearly 1 . Predictions of this fraction from MC simulation are sensitive to theoretical uncertainties such as the modelling of initial- and final-state radiation, as well as experimental uncertainties, especially that on the jet energy scale. To reduce the impact of these uncertainties, the top quark background determination uses data from a $b$-tagged control region in which the one-to-two jet ratio is compared to the MC simulation [112]. The resulting correction factor to a purely MC-based background estimate after all selections amounts to $1.11 \pm 0.06$ (stat).

In the 1 -jet and 2 -jet analyses, the top quark background predictions are normalised to the data using control samples defined by reversing the $b$-jet veto and removing the requirements on $\Delta \phi_{\ell \ell}$ and $m_{\ell \ell}$. The $\left|\Delta y_{\mathrm{jj}}\right|$ and $m_{\mathrm{jj}}$ requirements are included in the definition of the 2 -jet control region. The resulting samples are dominated by top quark events. The small contributions from other sources are taken into account using MC simulation and the data-driven $W+$ jets estimate. Good agreement between data and MC simulation is observed for the total numbers of events and the shapes of the $m_{\mathrm{T}}$ distributions. The resulting normalisation factors are $1.11 \pm 0.05$ for the 1 -jet control region and $1.01 \pm 0.26$ for the 2 -jet control region. Only the statistical uncertainties are quoted.

### 6.2.3. WW control sample

The MC predictions of the $W W$ background in the 0 -jet and 1-jet analyses, summed over lepton flavours, are normalised using control regions defined with the same selections as for the signal
region except that the $\Delta \phi_{\ell \ell}$ requirement is removed and the upper bound on $m_{\ell \ell}$ is replaced with a lower bound: $m_{\ell \ell}>80 \mathrm{GeV}$. The numbers of events and the shape of the $m_{\mathrm{T}}$ distribution in the control regions are in good agreement between data and MC, as shown in Fig. 5(b). WW production contributes about $70 \%$ of the events in the 0 -jet control region and about $45 \%$ in the 1 -jet region. Contaminations from sources other than $W W$ are derived as for the signal region, including the data-driven $W+$ jets and top estimates. The resulting normalisation factors with their associated statistical uncertainties are $1.06 \pm 0.06$ for the 0 -jet control region and $0.99 \pm 0.15$ for the 1 -jet control region.

### 6.3. Systematic uncertainties

The systematic uncertainties that have the largest impact on the sensitivity of the search are the theoretical uncertainties associated with the signal. These are described in Section 9. The main experimental uncertainties are associated with the JES, the jet energy resolution (JER), pile-up, $E_{\mathrm{T}}^{\text {miss }}$, the $b$-tagging efficiency, the $W+$ jets transfer factor, and the integrated luminosity. The largest uncertainties on the backgrounds include $W W$ normalisation and modelling, top normalisation, and $W \gamma^{(*)}$ normalisation. The 2-jet systematic uncertainties are dominated by the statistical uncertainties in the data and the MC simulation, and are therefore not discussed further.

Variations of the jet energy scale within the systematic uncertainties can cause events to migrate between the jet bins. The uncertainty on the JES varies from $\pm 2 \%$ to $\pm 9 \%$ as a function of jet $p_{\mathrm{T}}$ and $\eta$ for jets with $p_{\mathrm{T}}>25 \mathrm{GeV}$ and $|\eta|<4.5$ [101]. The largest impact of this uncertainty on the total signal (background) yield amounts to $7 \%(4 \%)$ in the 0 -jet (1-jet) bin. The uncertainty on the JER is estimated from in situ measurements and it impacts mostly the 1-jet channel, where its effect on the total signal and background yields is $4 \%$ and $2 \%$, respectively. An additional contribution to the JES uncertainty arises from pile-up, and is estimated to vary between $\pm 1 \%$ and $\pm 5 \%$ for multiple $p p$ collisions in the same bunch crossing and up to $\pm 10 \%$ for neighbouring bunch crossings. This uncertainty affects mainly the 1 -jet channel, where its impact on the signal and background yields is $4 \%$ and $2 \%$, respectively. JES and lepton momentum scale uncertainties are propagated to the $E_{\mathrm{T}}^{\text {miss }}$ measurement. Additional contributions to the $E_{\mathrm{T}}^{\text {miss }}$ uncertainties arise from jets with $p_{\mathrm{T}}<20 \mathrm{GeV}$ and from low-energy calorimeter deposits not associated with reconstructed physics objects [113]. The impact of the $E_{\mathrm{T}}^{\text {miss }}$ uncertainty on the total signal and background yields is $\sim 3 \%$. The efficiency of the $b$-tagging algorithm is calibrated using samples containing muons reconstructed in the vicinity of jets [114]. The uncertainty on the $b$-jet tagging efficiency varies between $\pm 5 \%$ and $\pm 18 \%$ as a function of the jet $p_{\mathrm{T}}$, and its impact on the total background yield is $10 \%$ for the 1 -jet channel. The uncertainty in the $W+$ jets transfer factor is dominated by differences in jet properties between dijet and $W+$ jets events as observed in MC simulations. The total uncertainty on this background is approximately $\pm 40 \%$, resulting in an uncertainty on the total background yield of $5 \%$. The uncertainty on the integrated luminosity is $\pm 3.6 \%$.

A fit to the distribution of $m_{\mathrm{T}}$ is performed in order to obtain the signal yield for each mass hypothesis (see Section 6.4). Most theoretical and experimental uncertainties do not produce statistically significant changes to the $m_{\mathrm{T}}$ distribution. The uncertainties that do produce significant changes of the distribution of $m_{\mathrm{T}}$ have no appreciable effect on the final results, with the exception of those associated with the $W W$ background. In this case, an uncertainty is included to take into account differences in the distribution of $m_{\mathrm{T}}$ and normalisation observed between the MCFM [115], MC@NLO + HERWIG and POWHEG + PYTHIA

Table 5
The expected numbers of signal ( $m_{H}=125 \mathrm{GeV}$ ) and background events after all selections, including a cut on the transverse mass of $0.75 m_{H}<m_{\mathrm{T}}<m_{H}$ for $m_{H}=$ 125 GeV . The observed numbers of events in data are also displayed. The $e \mu$ and $\mu e$ channels are combined. The uncertainties shown are the combination of the statistical and all systematic uncertainties, taking into account the constraints from control samples. For the 2 -jet analysis, backgrounds with fewer than 0.01 expected events are marked with '-'.

|  | 0 -jet | 1-jet | 2-jet |
| :--- | :--- | :--- | :--- |
| Signal | $20 \pm 4$ | $5 \pm 2$ | $0.34 \pm 0.07$ |
| $W W$ | $101 \pm 13$ | $12 \pm 5$ | $0.10 \pm 0.14$ |
| $W Z^{(*)} / Z Z / W \gamma^{(*)}$ | $12 \pm 3$ | $1.9 \pm 1.1$ | $0.10 \pm 0.10$ |
| $t \bar{t}$ | $8 \pm 2$ | $6 \pm 2$ | $0.15 \pm 0.10$ |
| $t W / t b / t q b$ | $3.4 \pm 1.5$ | $3.7 \pm 1.6$ | - |
| $Z / \gamma^{*}+$ jets | $1.9 \pm 1.3$ | $0.10 \pm 0.10$ | - |
| $W+$ jets | $15 \pm 7$ | $2 \pm 1$ | - |
| Total background | $142 \pm 16$ | $26 \pm 6$ | $0.35 \pm 0.18$ |
| Observed | 185 | 38 | 0 |

generators. The potential impact of interference between resonant (Higgs-mediated) and non-resonant $g g \rightarrow W W$ diagrams [116] for $m_{\mathrm{T}}>m_{H}$ was investigated and found to be negligible. The effect of the $W W$ normalisation, modelling, and shape systematics on the total background yield is $9 \%$ for the 0 -jet channel and $19 \%$ for the 1 -jet channel. The uncertainty on the shape of the total background is dominated by the uncertainties on the normalisations of the individual backgrounds. The main uncertainties on the top background in the 0 -jet analysis include those associated with interference effects between $t \bar{t}$ and single top, initial state an final state radiation, $b$-tagging, and JER. The impact on the total background yield in the 0 -jet bin is $3 \%$. For the 1 -jet analysis, the impact of the top background on the total yield is $14 \%$. Theoretical uncertainties on the $W \gamma$ background normalisation are evaluated for each jet bin using the procedure described in Ref. [117]. They are $\pm 11 \%$ for the 0 -jet bin and $\pm 50 \%$ for the 1 -jet bin. For $W \gamma^{*}$ with $m_{\ell \ell}<7 \mathrm{GeV}$, a $k$-factor of $1.3 \pm 0.3$ is applied to the MadGraph LO prediction based on the comparison with the MCFM NLO calculation. The $k$-factor for $W \gamma^{*} / W Z^{(*)}$ with $m_{\ell \ell}>7 \mathrm{GeV}$ is $1.5 \pm 0.5$. These uncertainties affect mostly the 1-jet channel, where their impact on the total background yield is approximately 4\%.

### 6.4. Results

Table 5 shows the numbers of events expected from a SM Higgs boson with $m_{H}=125 \mathrm{GeV}$ and from the backgrounds, as well as the numbers of candidates observed in data, after application of all selection criteria plus an additional cut on $m_{\mathrm{T}}$ of $0.75 m_{H}<m_{\mathrm{T}}<m_{H}$. The uncertainties shown in Table 5 include the systematic uncertainties discussed in Section 6.3, constrained by the use of the control regions discussed in Section 6.2. An excess of events relative to the background expectation is observed in the data.

Fig. 6 shows the distribution of the transverse mass after all selection criteria in the 0 -jet and 1 -jet channels combined, and for both lepton channels together.

The statistical analysis of the data employs a binned likelihood function constructed as the product of Poisson probability terms for the $e \mu$ channel and the $\mu e$ channel. The mass-dependent cuts on $m_{\mathrm{T}}$ described above are not used. Instead, the 0 -jet (1-jet) signal regions are subdivided into five (three) $m_{\mathrm{T}}$ bins. For the 2-jet signal region, only the results integrated over $m_{\mathrm{T}}$ are used, due to the small number of events in the final sample. The statistical interpretation of the observed excess of events is presented in Section 9.


Fig. 6. Distribution of the transverse mass, $m_{\mathrm{T}}$, in the 0 -jet and 1 -jet analyses with both $e \mu$ and $\mu e$ channels combined, for events satisfying all selection criteria. The expected signal for $m_{H}=125 \mathrm{GeV}$ is shown stacked on top of the background prediction. The $W+$ jets background is estimated from data, and $W W$ and top background MC predictions are normalised to the data using control regions. The hashed area indicates the total uncertainty on the background prediction.

## 7. Statistical procedure

The statistical procedure used to interpret the data is described in Refs. [17,118-121]. The parameter of interest is the global signal strength factor $\mu$, which acts as a scale factor on the total number of events predicted by the Standard Model for the Higgs boson signal. This factor is defined such that $\mu=0$ corresponds to the background-only hypothesis and $\mu=1$ corresponds to the SM Higgs boson signal in addition to the background. Hypothesised values of $\mu$ are tested with a statistic $\lambda(\mu)$ based on the profile likelihood ratio [122]. This test statistic extracts the information on the signal strength from a full likelihood fit to the data. The likelihood function includes all the parameters that describe the systematic uncertainties and their correlations.

Exclusion limits are based on the $C L_{s}$ prescription [123]; a value of $\mu$ is regarded as excluded at $95 \% \mathrm{CL}$ when $C L_{s}$ is less than $5 \%$. A SM Higgs boson with mass $m_{H}$ is considered excluded at $95 \%$ confidence level (CL) when $\mu=1$ is excluded at that mass. The significance of an excess in the data is first quantified with the local $p_{0}$, the probability that the background can produce a fluctuation greater than or equal to the excess observed in data. The equivalent formulation in terms of number of standard deviations, $Z_{l}$, is referred to as the local significance. The global probability for the most significant excess to be observed anywhere in a given search region is estimated with the method described in Ref. [124]. The ratio of the global to the local probabilities, the trials factor used to correct for the "look elsewhere" effect, increases with the range of Higgs boson mass hypotheses considered, the mass resolutions of the channels involved in the combination, and the significance of the excess.

The statistical tests are performed in steps of values of the hypothesised Higgs boson mass $m_{H}$. The asymptotic approximation [122] upon which the results are based has been validated with the method described in Ref. [17].

The combination of individual search sub-channels for a specific Higgs boson decay, and the full combination of all search channels, are based on the global signal strength factor $\mu$ and on the identification of the nuisance parameters that correspond to the correlated sources of systematic uncertainty described in Section 8.

## 8. Correlated systematic uncertainties

The individual search channels that enter the combination are summarised in Table 6.

Table 6

 requirements, respectively.

| Higgs boson decay | Subsequent decay | Sub-channels | $m_{H}$ range [GeV] | $\int \mathrm{Ldt}\left[\mathrm{fb}^{-1}\right]$ | Ref. |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $2011 \sqrt{s}=7 \mathrm{TeV}$ |  |  |  |  |  |
| $H \rightarrow Z Z^{(*)}$ | $4 \ell$ | $\{4 e, 2 e 2 \mu, 2 \mu 2 e, 4 \mu\}$ | 110-600 | 4.8 | [87] |
|  | $\ell \ell \nu \bar{v}$ | \{ee, $\mu \mu\} \otimes$ low, high pile-up\} | 200-280-600 | 4.7 | [125] |
|  | $\ell \ell q \bar{q}$ | \{b-tagged, untagged $\}$ | 200-300-600 | 4.7 | [126] |
| $H \rightarrow \gamma \gamma$ | - | 10 categories $\left\{p_{\mathrm{Tt}} \otimes \eta_{\gamma} \otimes\right.$ conversion $\} \oplus\{2$-jet $\}$ | 110-150 | 4.8 | [127] |
| $H \rightarrow W W^{(*)}$ | $\ell \nu \ell \nu$ | $\{e e, e \mu / \mu e, \mu \mu\} \otimes\{0$-jet, 1-jet, 2-jet $\} \otimes\{$ low, high pile-up $\}$ | 110-200-300-600 | 4.7 | [106] |
|  | $\ell \nu q q^{\prime}$ | $\{e, \mu\} \otimes\{0$-jet, 1 -jet, 2 -jet $\}$ | 300-600 | 4.7 | [128] |
| $H \rightarrow \tau \tau$ | $\tau_{\text {lep }} \tau_{\text {lep }}$ | $\{e \mu\} \otimes\{0$-jet $\} \oplus\{\ell \ell\} \otimes\{1$-jet, 2-jet, $V H\}$ | 110-150 | 4.7 | [129] |
|  | $\tau_{\text {lep }} \tau_{\text {had }}$ | $\{e, \mu\} \otimes\{0 \text {-jet }\} \otimes\left\{E_{\mathrm{T}}^{\text {miss }}<20 \mathrm{GeV}, E_{\mathrm{T}}^{\text {miss }} \geqslant 20 \mathrm{GeV}\right\}$ $\oplus\{e, \mu\} \otimes\{1$-jet $\} \oplus\{\ell\} \otimes\{2$-jet $\}$ | 110-150 | 4.7 |  |
|  | $\tau_{\text {had }} \tau_{\text {had }}$ | \{1-jet $\}$ | 110-150 | 4.7 |  |
| $V H \rightarrow V b b$ | $Z \rightarrow \nu \nu$ | $E_{\mathrm{T}}^{\text {miss }} \in\{120-160,160-200, \geqslant 200 \mathrm{GeV}\}$ | 110-130 | 4.6 | [130] |
|  | $W \rightarrow \ell \nu$ | $p_{\mathrm{T}}^{W} \in\{<50,50-100,100-200, \geqslant 200 \mathrm{GeV}\}$ | 110-130 | 4.7 |  |
|  | $Z \rightarrow \ell \ell$ | $p_{\mathrm{T}}^{Z} \in\{<50,50-100,100-200, \geqslant 200 \mathrm{GeV}\}$ | 110-130 | 4.7 |  |
| $2012 \sqrt{s}=8 \mathrm{TeV}$ |  |  |  |  |  |
| $H \rightarrow Z Z^{(*)}$ | $4 \ell$ | $\{4 e, 2 e 2 \mu, 2 \mu 2 e, 4 \mu\}$ | 110-600 | 5.8 | [87] |
| $H \rightarrow \gamma \gamma$ | - | 10 categories $\left\{p_{\mathrm{Tt}} \otimes \eta_{\gamma} \otimes\right.$ conversion $\} \oplus\{2$-jet $\}$ | 110-150 | 5.9 | [127] |
| $H \rightarrow W W^{(*)}$ | ev $\mu \nu$ | $\{e \mu, \mu e\} \otimes\{0$-jet, 1-jet, 2-jet $\}$ | 110-200 | 5.8 | [131] |

The main uncorrelated systematic uncertainties are described in Sections 4-6 for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow \gamma \gamma$ and $H \rightarrow$ $W W^{(*)} \rightarrow \ell \nu \ell \nu$ channels and in Ref. [17] for the other channels. They include the background normalisations or background model parameters from control regions or sidebands, the Monte Carlo simulation statistical uncertainties and the theoretical uncertainties affecting the background processes.

The main sources of correlated systematic uncertainties are the following.

1. Integrated luminosity: The uncertainty on the integrated luminosity is considered as fully correlated among channels and amounts to $\pm 3.9 \%$ for the 7 TeV data [132,133], except for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$ channels which were re-analysed; the uncertainty is $\pm 1.8 \%$ [92] for these channels. The uncertainty is $\pm 3.6 \%$ for the 8 TeV data.
2. Electron and photon trigger identification: The uncertainties in the trigger and identification efficiencies are treated as fully correlated for electrons and photons.
3. Electron and photon energy scales: The electron and photon energy scales in the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$ channels are described by five parameters, which provide a detailed account of the sources of systematic uncertainty. They are related to the calibration method, the presampler energy scale in the barrel and end-cap calorimeters, and the material description upstream of the calorimeters.
4. Muon reconstruction: The uncertainties affecting muons are separated into those related to the ID and MS, in order to obtain a better description of the correlated effects among channels using different muon identification criteria and different ranges of muon $p_{\mathrm{T}}$.
5. Jet energy scale and missing transverse energy: The jet energy scale and jet energy resolution are affected by uncertainties which depend on the $p_{\mathrm{T}}, \eta$, and flavour of the jet. A simplified scheme is used in which independent JES and JER nuisance parameters are associated with final states with significantly different kinematic selections and sensitivity to scattering processes with different kinematic distributions or flavour composition. This scheme includes a specific treatment for $b$-jets. The sensitivity of the results to various assumptions about the correlation between these sources of uncertainty has been found to be negligible. An uncorrelated component of the uncertainty on $E_{\mathrm{T}}^{\mathrm{miss}}$ is included, in
addition to the JES uncertainty, which is due to low energy jet activity not associated with reconstructed physics objects.
6. Theory uncertainties: Correlated theoretical uncertainties affect mostly the signal predictions. The QCD scale uncertainties for $m_{H}=125 \mathrm{GeV}$ amount to ${ }_{-8 \%}^{+7 \%}$ for the ggF process, $\pm 1 \%$ for the VBF and $W H / Z H$ processes, and ${ }_{-9 \%}^{+4 \%}$ for the $t \bar{t} H$ process [52,53]; the small dependence of these uncertainties on $m_{H}$ is taken into account. The uncertainties on the predicted branching ratios amount to $\pm 5 \%$. The uncertainties related to the parton distribution functions amount to $\pm 8 \%$ for the predominantly gluon-initiated ggF and $t \bar{t} H$ processes, and $\pm 4 \%$ for the predominantly quark-initiated VBF and $W H / Z H$ processes [78,134-136]. The theoretical uncertainty associated with the exclusive Higgs boson production process with additional jets in the $H \rightarrow \gamma \gamma, H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ and $H \rightarrow \tau^{+} \tau^{-}$channels is estimated using the prescription of Refs. [53,117,118], with the noticeable difference that an explicit calculation of the gluon-fusion process at NLO using MCFM [137] in the 2-jet category reduces the uncertainty on this non-negligible contribution to $25 \%$. An additional theoretical uncertainty on the signal normalisation of $\pm 150 \% \times\left(m_{H} / \mathrm{TeV}\right)^{3}$ (e.g. $\pm 4 \%$ for $m_{H}=$ 300 GeV ) accounts for effects related to off-shell Higgs boson production and interference with other SM processes [53].

Sources of systematic uncertainty that affect both the 7 TeV and the 8 TeV data are taken as fully correlated. The uncertainties on background estimates based on control samples in the data are considered uncorrelated between the 7 TeV and 8 TeV data.

## 9. Results

The addition of the 8 TeV data for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow$ $\gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ channels, as well as the improvements to the analyses of the 7 TeV data in the first two of these channels, bring a significant gain in sensitivity in the low-mass region with respect to the previous combined search [17].

### 9.1. Excluded mass regions

The combined 95\% CL exclusion limits on the production of the SM Higgs boson, expressed in terms of the signal strength parameter $\mu$, are shown in Fig. $7(\mathrm{a})$ as a function of $m_{H}$. The expected $95 \% \mathrm{CL}$ exclusion region covers the $m_{H}$ range from 110 GeV to


Fig. 7. Combined search results: (a) The observed (solid) $95 \%$ CL limits on the signal strength as a function of $m_{H}$ and the expectation (dashed) under the backgroundonly hypothesis. The dark and light shaded bands show the $\pm 1 \sigma$ and $\pm 2 \sigma$ uncertainties on the background-only expectation. (b) The observed (solid) local $p_{0}$ as a function of $m_{H}$ and the expectation (dashed) for a SM Higgs boson signal hypothesis $(\mu=1)$ at the given mass. (c) The best-fit signal strength $\hat{\mu}$ as a function of $m_{H}$. The band indicates the approximate $68 \%$ CL interval around the fitted value.

582 GeV . The observed $95 \%$ CL exclusion regions are $111-122 \mathrm{GeV}$ and $131-559 \mathrm{GeV}$. Three mass regions are excluded at $99 \% \mathrm{CL}$, $113-114,117-121$ and $132-527 \mathrm{GeV}$, while the expected exclusion range at $99 \% \mathrm{CL}$ is $113-532 \mathrm{GeV}$.

### 9.2. Observation of an excess of events

An excess of events is observed near $m_{H}=126 \mathrm{GeV}$ in the $H \rightarrow$ $Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$ channels, both of which provide fully reconstructed candidates with high resolution in invariant mass, as shown in Figs. 8(a) and 8(b). These excesses are confirmed by the highly sensitive but low-resolution $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channel, as shown in Fig. 8(c).

The observed local $p_{0}$ values from the combination of channels, using the asymptotic approximation, are shown as a function of $m_{H}$ in Fig. 7(b) for the full mass range and in Fig. 9 for the low mass range.

The largest local significance for the combination of the 7 and 8 TeV data is found for a SM Higgs boson mass hypothesis of $m_{H}=126.5 \mathrm{GeV}$, where it reaches $6.0 \sigma$, with an expected value in the presence of a SM Higgs boson signal at that mass of $4.9 \sigma$ (see also Table 7). For the 2012 data alone, the maximum local significance for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow \gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow$


Fig. 8. The observed local $p_{0}$ as a function of the hypothesised Higgs boson mass for the (a) $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$, (b) $H \rightarrow \gamma \gamma$ and (c) $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channels. The dashed curves show the expected local $p_{0}$ under the hypothesis of a SM Higgs boson signal at that mass. Results are shown separately for the $\sqrt{s}=7 \mathrm{TeV}$ data (dark, blue in the web version), the $\sqrt{s}=8 \mathrm{TeV}$ data (light, red in the web version), and their combination (black).


Fig. 9. The observed (solid) local $p_{0}$ as a function of $m_{H}$ in the low mass range. The dashed curve shows the expected local $p_{0}$ under the hypothesis of a SM Higgs boson signal at that mass with its $\pm 1 \sigma$ band. The horizontal dashed lines indicate the $p$-values corresponding to significances of 1 to $6 \sigma$.
$e \nu \mu \nu$ channels combined is $4.9 \sigma$, and occurs at $m_{H}=126.5 \mathrm{GeV}$ (3.8 $\sigma$ expected).

The significance of the excess is mildly sensitive to uncertainties in the energy resolutions and energy scale systematic uncertainties for photons and electrons; the effect of the muon energy scale systematic uncertainties is negligible. The presence of these

Table 7
Characterisation of the excess in the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow \gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channels and the combination of all channels listed in Table 6 . The mass value $m_{\max }$ for which the local significance is maximum, the maximum observed local significance $Z_{l}$ and the expected local significance $E\left(Z_{l}\right)$ in the presence of a SM Higgs boson signal at $m_{\max }$ are given. The best fit value of the signal strength parameter $\hat{\mu}$ at $m_{H}=126 \mathrm{GeV}$ is shown with the total uncertainty. The expected and observed mass ranges excluded at $95 \% \mathrm{CL}\left(99 \% \mathrm{CL}\right.$, indicated by a ${ }^{*}$ ) are also given, for the combined $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data.

| Search channel | Dataset | $m_{\text {max }}[\mathrm{GeV}]$ | $Z_{l}[\sigma]$ | $E\left(Z_{l}\right)[\sigma]$ | $\hat{\mu}\left(m_{H}=126 \mathrm{GeV}\right)$ | Expected exclusion [GeV] | Observed exclusion [GeV] |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ | 7 TeV | 125.0 | 2.5 | 1.6 | $1.4 \pm 1.1$ |  |  |
|  | 8 TeV | 125.5 | 2.6 | 2.1 | $1.1 \pm 0.8$ |  |  |
|  | $7 \& 8 \mathrm{TeV}$ | 125.0 | 3.6 | 2.7 | $1.2 \pm 0.6$ | 124-164, 176-500 | 131-162, 170-460 |
| $H \rightarrow \gamma \gamma$ | 7 TeV | 126.0 | 3.4 | 1.6 | $2.2 \pm 0.7$ |  |  |
|  | 8 TeV | 127.0 | 3.2 | 1.9 | $1.5 \pm 0.6$ |  |  |
|  | 7 \& 8 TeV | 126.5 | 4.5 | 2.5 | $1.8 \pm 0.5$ | 110-140 | 112-123, 132-143 |
| $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ | 7 TeV | 135.0 | 1.1 | 3.4 | $0.5 \pm 0.6$ |  |  |
|  | 8 TeV | 120.0 | 3.3 | 1.0 | $1.9 \pm 0.7$ |  |  |
|  | 7 \& 8 TeV | 125.0 | 2.8 | 2.3 | $1.3 \pm 0.5$ | 124-233 | 137-261 |
| Combined | 7 TeV | 126.5 | 3.6 | 3.2 | $1.2 \pm 0.4$ |  |  |
|  | 8 TeV | 126.5 | 4.9 | 3.8 | $1.5 \pm 0.4$ |  |  |
|  | $7 \& 8 \mathrm{TeV}$ | 126.5 | 6.0 | 4.9 | $1.4 \pm 0.3$ | $\begin{aligned} & 110-582 \\ & 113-532 \text { (*) }^{*} \end{aligned}$ | $\begin{aligned} & 111-122,131-559 \\ & 113-114,117-121,132-527 \text { (*) }^{*} \end{aligned}$ |

uncertainties, evaluated as described in Ref. [138], reduces the local significance to $5.9 \sigma$.

The global significance of a local $5.9 \sigma$ excess anywhere in the mass range $110-600 \mathrm{GeV}$ is estimated to be approximately $5.1 \sigma$, increasing to $5.3 \sigma$ in the range $110-150 \mathrm{GeV}$, which is approximately the mass range not excluded at the $99 \%$ CL by the LHC combined SM Higgs boson search [139] and the indirect constraints from the global fit to precision electroweak measurements [12].

### 9.3. Characterising the excess

The mass of the observed new particle is estimated using the profile likelihood ratio $\lambda\left(m_{H}\right)$ for $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$, the two channels with the highest mass resolution. The signal strength is allowed to vary independently in the two channels, although the result is essentially unchanged when restricted to the SM hypothesis $\mu=1$. The leading sources of systematic uncertainty come from the electron and photon energy scales and resolutions. The resulting estimate for the mass of the observed particle is $126.0 \pm 0.4$ (stat) $\pm 0.4$ (sys) GeV .

The best-fit signal strength $\hat{\mu}$ is shown in Fig. 7(c) as a function of $m_{H}$. The observed excess corresponds to $\hat{\mu}=1.4 \pm 0.3$ for $m_{H}=$ 126 GeV , which is consistent with the SM Higgs boson hypothesis $\mu=1$. A summary of the individual and combined best-fit values of the strength parameter for a SM Higgs boson mass hypothesis of 126 GeV is shown in Fig. 10, while more information about the three main channels is provided in Table 7.

In order to test which values of the strength and mass of a signal hypothesis are simultaneously consistent with the data, the profile likelihood ratio $\lambda\left(\mu, m_{H}\right)$ is used. In the presence of a strong signal, it will produce closed contours around the best-fit point $\left(\hat{\mu}, \hat{m}_{H}\right)$, while in the absence of a signal the contours will be upper limits on $\mu$ for all values of $m_{H}$.

Asymptotically, the test statistic $-2 \ln \lambda\left(\mu, m_{H}\right)$ is distributed as a $\chi^{2}$ distribution with two degrees of freedom. The resulting $68 \%$ and $95 \% \mathrm{CL}$ contours for the $H \rightarrow \gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channels are shown in Fig. 11, where the asymptotic approximations have been validated with ensembles of pseudo-experiments. Similar contours for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ channel are also shown in Fig. 11, although they are only approximate confidence intervals due to the smaller number of candidates in this channel. These contours in the $\left(\mu, m_{H}\right)$ plane take into account uncertainties in the energy scale and resolution.

The probability for a single Higgs boson-like particle to produce resonant mass peaks in the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$


Fig. 10. Measurements of the signal strength parameter $\mu$ for $m_{H}=126 \mathrm{GeV}$ for the individual channels and their combination.


Fig. 11. Confidence intervals in the $\left(\mu, m_{H}\right)$ plane for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow$ $\gamma \gamma$, and $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channels, including all systematic uncertainties. The markers indicate the maximum likelihood estimates $\left(\hat{\mu}, \hat{m}_{H}\right)$ in the corresponding channels (the maximum likelihood estimates for $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ coincide).
channels separated by more than the observed mass difference, allowing the signal strengths to vary independently, is about $8 \%$.

The contributions from the different production modes in the $H \rightarrow \gamma \gamma$ channel have been studied in order to assess any tension between the data and the ratios of the production cross


Fig. 12. Likelihood contours for the $H \rightarrow \gamma \gamma$ channel in the $\left(\mu_{\mathrm{ggF}+t \bar{t} H}, \mu_{\mathrm{VBF}+V H}\right)$ plane including the branching ratio factor $B / B_{S M}$. The quantity $\mu_{\mathrm{ggF}+t \bar{t} H}^{\mathrm{g}}\left(\mu_{\mathrm{VBF}+V H}\right)$ is a common scale factor for the ggF and $t \bar{t} H$ (VBF and $V H$ ) production cross sections. The best fit to the data ( + ) and $68 \%$ (full) and $95 \%$ (dashed) CL contours are also indicated, as well as the SM expectation ( $\times$ ).
sections predicted in the Standard Model. A new signal strength parameter $\mu_{i}$ is introduced for each production mode, defined by $\mu_{i}=\sigma_{i} / \sigma_{i, \mathrm{SM}}$. In order to determine the values of ( $\mu_{i}, \mu_{j}$ ) that are simultaneously consistent with the data, the profile likelihood ratio $\lambda\left(\mu_{i}, \mu_{j}\right)$ is used with the measured mass treated as a nuisance parameter.

Since there are four Higgs boson production modes at the LHC, two-dimensional contours require either some $\mu_{i}$ to be fixed, or multiple $\mu_{i}$ to be related in some way. Here, $\mu_{\text {ggF }}$ and $\mu_{t \bar{t} H}$ have been grouped together as they scale with the $t \bar{t} H$ coupling in the SM, and are denoted by the common parameter $\mu_{\text {ggF }+t \bar{t} H}$. Similarly, $\mu_{\mathrm{VBF}}$ and $\mu_{V H}$ have been grouped together as they scale with the $W W H / Z Z H$ coupling in the SM, and are denoted by the common parameter $\mu_{\mathrm{VBF}+V H}$. Since the distribution of signal events among the 10 categories of the $H \rightarrow \gamma \gamma$ search is sensitive to these factors, constraints in the plane of $\mu_{\mathrm{ggF}+\mathrm{t} \overline{\mathrm{H}} \mathrm{H}} \times B / B_{\mathrm{SM}}$ and $\mu_{\mathrm{VBF}+V H} \times B / B_{\mathrm{SM}}$, where $B$ is the branching ratio for $H \rightarrow \gamma \gamma$, can be obtained (Fig. 12). Theoretical uncertainties are included so that the consistency with the SM expectation can be quantified. The data are compatible with the SM expectation at the $1.5 \sigma$ level.

## 10. Conclusion

Searches for the Standard Model Higgs boson have been performed in the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell, H \rightarrow \gamma \gamma$ and $H \rightarrow W W^{(*)} \rightarrow$ $e \nu \mu \nu$ channels with the ATLAS experiment at the LHC using 5.8$5.9 \mathrm{fb}^{-1}$ of $p p$ collision data recorded during April to June 2012 at a centre-of-mass energy of 8 TeV . These results are combined with earlier results [17], which are based on an integrated luminosity of $4.6-4.8 \mathrm{fb}^{-1}$ recorded in 2011 at a centre-of-mass energy of 7 TeV , except for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$ channels, which have been updated with the improved analyses presented here.

The Standard Model Higgs boson is excluded at 95\% CL in the mass range $111-559 \mathrm{GeV}$, except for the narrow region 122131 GeV . In this region, an excess of events with significance $5.9 \sigma$, corresponding to $p_{0}=1.7 \times 10^{-9}$, is observed. The excess is driven by the two channels with the highest mass resolution, $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$, and the equally sensitive but lowresolution $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channel. Taking into account the entire mass range of the search, $110-600 \mathrm{GeV}$, the global significance of the excess is $5.1 \sigma$, which corresponds to $p_{0}=1.7 \times 10^{-7}$.

These results provide conclusive evidence for the discovery of a new particle with mass $126.0 \pm 0.4$ (stat) $\pm 0.4$ (sys) GeV . The signal strength parameter $\mu$ has the value $1.4 \pm 0.3$ at the fitted mass,
which is consistent with the SM Higgs boson hypothesis $\mu=1$. The decays to pairs of vector bosons whose net electric charge is zero identify the new particle as a neutral boson. The observation in the diphoton channel disfavours the spin- 1 hypothesis [140, 141]. Although these results are compatible with the hypothesis that the new particle is the Standard Model Higgs boson, more data are needed to assess its nature in detail.

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# Measurement of the inclusive isolated prompt photon cross section in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

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#### Abstract

A measurement of the cross section for the inclusive production of isolated prompt photons in $p p$ collisions at a center-of-mass energy $\sqrt{s}=7 \mathrm{TeV}$ is presented. The measurement covers the pseudorapidity ranges $\left|\eta^{\gamma}\right|<1.37$ and $1.52 \leq\left|\eta^{\gamma}\right|<1.81$ in the transverse energy range $15 \leq E_{\mathrm{T}}^{\gamma}<100 \mathrm{GeV}$. The results are based on an integrated luminosity of $880 \mathrm{nb}^{-1}$, collected with the ATLAS detector at the Large Hadron Collider. Photon candidates are identified by combining information from the calorimeters and from the inner tracker. Residual background in the selected sample is estimated from data based on the observed distribution of the transverse isolation energy in a narrow cone around the photon candidate. The results are compared to predictions from next-to-leading-order perturbative QCD calculations.


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## I. INTRODUCTION

Prompt photon production at hadron colliders provides a handle for testing perturbative QCD (pQCD) predictions [1,2]. Photons provide a colorless probe of quarks in the hard partonic interaction and the subsequent partonshower. Their production is directly sensitive to the gluon content of the proton through the $q g \rightarrow q \gamma$ process, which dominates at leading-order (LO). The measurement of the prompt photon production cross section can thus be exploited to constrain the gluon density function [3,4]. Furthermore, photon identification is important for many physics signatures, including searches for Higgs boson [5] and graviton decays [6] to photon pairs, decays of excited fermions [7], and decays of pairs of supersymmetric particles characterized by the production of two energetic photons and large missing transverse energy [8-10].

Prompt photons include both "direct" photons, which take part in the hard scattering subprocess (mostly quarkgluon Compton scattering, $q g \rightarrow q \gamma$, or quark-antiquark annihilation, $q \bar{q} \rightarrow g \gamma$ ), and "fragmentation" photons, which are the result of the fragmentation of a high- $p_{T}$ parton [11,12]. In this analysis, an isolation criterion is applied based on the amount of transverse energy inside a cone of radius $R=\sqrt{\left(\eta-\eta^{\gamma}\right)^{2}+\left(\phi-\phi^{\gamma}\right)^{2}}=0.4$ centered around the photon direction in the pseudorapidity $(\eta)$ and azimuthal angle ( $\phi$ ) plane [13]. After the isolation requirement is applied the relative contribution to the total cross section from fragmentation photons decreases, though it remains non-negligible especially at low
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transverse energies [12]. The isolation requirement also significantly reduces the main background of nonprompt photon candidates from decays of energetic $\pi^{0}$ and $\eta$ mesons inside jets.

Early studies of prompt photon production were carried out at the ISR collider [14,15]. Subsequent studies, for example [16-18], further established prompt photons as a useful probe of parton interactions. More recent measurements at hadron colliders were performed at the Tevatron, in $p \bar{p}$ collisions at a center-of-mass energy $\sqrt{s}=1.96 \mathrm{TeV}$. The measurement by the D 0 Collaboration [19] is based on $326 \mathrm{pb}^{-1}$ and covers a pseudorapidity range $\left|\eta^{\gamma}\right|<0.9$ and a transverse energy range $23<E_{\mathrm{T}}^{\gamma}<300 \mathrm{GeV}$, while the measurement by the CDF Collaboration [20] is based on $2.5 \mathrm{fb}^{-1}$ and covers a pseudorapidity range $\left|\eta^{\gamma}\right|<1.0$ and a transverse energy range $30<E_{\mathrm{T}}^{\gamma}<400 \mathrm{GeV}$. Both D0 and CDF measure an isolated prompt photon cross section in agreement with next-to-leading-order (NLO) pQCD calculations, with a slight excess seen in the CDF data between 30 and 50 GeV . Measurements of the inclusive prompt photon production cross section have also been performed in ep collisions, both in photoproduction and deep inelastic scattering, by the H1 [21,22] and ZEUS [23,24] Collaborations. The most recent measurement of the inclusive isolated prompt photon production was done with $2.9 \mathrm{pb}^{-1}$ at $\sqrt{s}=7 \mathrm{TeV}$ by the CMS Collaboration [25]. That measurement, which covers $21<E_{\mathrm{T}}^{\gamma}<$ 300 GeV and $\left|\eta^{\gamma}\right|<1.45$, is in good agreement with NLO predictions for the full $E_{\mathrm{T}}^{\gamma}$ range.

This paper describes the extraction of a signal of isolated prompt photons using $880 \mathrm{nb}^{-1}$ of data collected with the ATLAS detector at the Large Hadron Collider (LHC). A measurement of the production cross section in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ is presented, in the pseudorapidity ranges $\left|\eta^{\gamma}\right|<0.6,0.6 \leq\left|\eta^{\gamma}\right|<1.37$ and $1.52 \leq\left|\eta^{\gamma}\right|<$ 1.81, for photons with transverse energies between 15 GeV and 100 GeV .

The paper is organized as follows. The detector is described in Sec. II, followed by a summary of the data and the simulated samples used in the measurement in Sec. III. Section IV introduces the theoretical predictions to which the measurement is compared. Section V describes the photon reconstruction and identification algorithms; their performance is given in Sec. VI. Section VII describes the methods used to estimate the residual background in the data and to extract the prompt photon signal, followed by a discussion of the data corrections for the cross section measurement in Sec. VIII. The sources of systematic uncertainties on the cross section measurement are discussed in Sec. IX. Section X contains the main experimental results and the comparison of the observed cross sections with the theoretical predictions, followed by the conclusions in Sec. XI.

## II. THE ATLAS DETECTOR

The ATLAS detector is described in detail in Refs. [26,27]. For the measurement presented in this paper, the calorimeter, with mainly its electromagnetic section, and the inner detector are of particular relevance.

The inner detector consists of three subsystems: at small radial distance $r$ from the beam axis ( $50.5<r<150 \mathrm{~mm}$ ), pixel silicon detectors are arranged in three cylindrical layers in the barrel and in three disks in each end-cap; at intermediate radii ( $299<r<560 \mathrm{~mm}$ ), double layers of single-sided silicon microstrip detectors are used, organized in four cylindrical layers in the barrel and nine disks in each end-cap; at larger radii $(563<r<1066 \mathrm{~mm})$, a straw tracker with transition-radiation detection capabilities divided into one barrel section (with 73 layers of straws parallel to the beam line) and two end-caps (with 160 layers each of straws radial to the beam line) is used. These three systems are immersed in a 2 T axial magnetic field provided by a superconducting solenoid. The inner detector has full coverage in $\phi$. The silicon pixel and microstrip subsystems cover the pseudorapidity range $|\eta|<2.5$, while the transition-radiation tracker acceptance is limited to the range $|\eta|<2.0$. The inner detector allows an accurate reconstruction of tracks from the primary proton-proton collision region, and also identifies tracks from secondary vertices, permitting the efficient reconstruction of photon conversions in the inner detector up to a radius of $\approx 80 \mathrm{~cm}$.

The electromagnetic calorimeter is a lead-liquid argon ( $\mathrm{Pb}-\mathrm{LAr}$ ) sampling calorimeter with an accordion geometry. It is divided into a barrel section, covering the pseudorapidity region $|\eta|<1.475$, and two end-cap sections, covering the pseudorapidity regions $1.375<|\eta|<3$.2. It consists of three longitudinal layers. The first one, with a thickness between 3 and 5 radiation lengths, is segmented into high granularity strips in the $\eta$ direction (width between 0.003 and 0.006 depending on $\eta$, with the exception of the regions $1.4<|\eta|<1.5$ and $|\eta|>2.4$ ), sufficient to
provide an event-by-event discrimination between singlephoton showers and two overlapping showers coming from a $\pi^{0}$ decay. The second layer of the electromagnetic calorimeter, which collects most of the energy deposited in the calorimeter by the photon shower, has a thickness around 17 radiation lengths and a granularity of $0.025 \times 0.025$ in $\eta \times \phi$ (corresponding to one cell). A third layer, with thickness varying between 4 and 15 radiation lengths, is used to correct leakage beyond the calorimeter for highenergy showers. In front of the accordion calorimeter a thin presampler layer, covering the pseudorapidity interval $|\eta|<1.8$, is used to correct for energy loss before the calorimeter. The sampling term $a$ of the energy resolution $(\sigma(E) / E \approx a / \sqrt{E[\mathrm{GeV}]})$ varies between $10 \%$ and $17 \%$ as a function of $|\eta|$ and is the largest contribution to the resolution up to about 200 GeV , where the global constant term, estimated to be $0.7 \%$ [28], starts to dominate.

The total amount of material before the first active layer of the electromagnetic calorimeter (including the presampler) varies between 2.5 and 6 radiation lengths as a function of pseudorapidity, excluding the transition region ( $1.37 \leq|\eta|<1.52$ ) between the barrel and the end-caps, where the material thickness increases to 11.5 radiation lengths. The central region $(|\eta|<0.6)$ has significantly less material than the outer barrel $(0.6 \leq|\eta|<1.37)$, which motivates the division of the barrel into two separate regions in pseudorapidity.

A hadronic sampling calorimeter is located beyond the electromagnetic calorimeter. It is made of steel and scintillating tiles in the barrel section $(|\eta|<1.7)$, with depth around 7.4 interaction lengths, and of two end-caps of copper and liquid argon, with depth around 9 interaction lengths.

A three-level trigger system is used to select events containing photon candidates during data-taking [29]. The first level trigger (level-1) is hardware based: using a coarser cell granularity ( $0.1 \times 0.1$ in $\eta \times \phi$ ) than that of the electromagnetic calorimeter, it searches for electromagnetic clusters within a fixed window of size $0.2 \times 0.2$ and retains only those whose total transverse energy in two adjacent cells is above a programmable threshold. The second and third level triggers (collectively referred to as the "high-level" trigger) are implemented in software. The high-level trigger exploits the full granularity and precision of the calorimeter to refine the level-1 trigger selection, based on improved energy resolution and detailed information on energy deposition in the calorimeter cells.

## III. COLLISION DATA AND SIMULATED SAMPLES

## A. Collision data

The measurement presented here is based on protonproton collision data collected at a center-of-mass energy $\sqrt{s}=7 \mathrm{TeV}$ between April and August 2010. Events in
which the calorimeters or the inner detector are not fully operational, or show data quality problems, are excluded. Events are triggered using a single-photon high-level trigger with a nominal transverse energy threshold of 10 GeV , seeded by a level-1 trigger with nominal threshold equal to 5 GeV . The selection criteria applied by the trigger on shower-shape variables computed from the energy profiles of the showers in the calorimeters are looser than the photon identification criteria applied in the offline analysis, and allow ATLAS to reach a plateau of constant efficiency close to $100 \%$ for true prompt photons with $E_{\mathrm{T}}^{\gamma}>15 \mathrm{GeV}$ and pseudorapidity $\left|\eta^{\gamma}\right|<1.81$. In addition, samples of minimum-bias events, triggered by using two sets of scintillator counters located at $z= \pm 3.5 \mathrm{~m}$ from the collision center, are used to estimate the single-photon trigger efficiency. The total integrated luminosity of the sample passing data quality and trigger requirements amounts to $(880 \pm 100) \mathrm{nb}^{-1}$.

In order to reduce noncollision backgrounds, events are required to have at least one reconstructed primary vertex consistent with the average beam spot position and with at least three associated tracks. The efficiency of this requirement is expected to be greater than $99.9 \%$ in events containing a prompt photon with $E_{\mathrm{T}}^{\gamma}>15 \mathrm{GeV}$ and lying within the calorimeter acceptance. The total number of selected events in data after this requirement is $9.6 \times$ $10^{6}$. The remaining amount of noncollision background is estimated using control samples collectedduring normal data-taking conditions-with dedicated, low threshold triggers that are activated in events where either no proton bunch or only one of the two beams crosses the interaction region. The estimated contribution to the final photon sample is less than $0.1 \%$ and is therefore neglected.

## B. Simulated events

To study the characteristics of signal and background events, Monte Carlo (MC) samples are generated using PYTHIA 6.4.21 [30], a leading-order parton-shower MC generator, with the modified leading-order MRST2007 [31] parton distribution functions (PDFs). It accounts for QED radiation emitted off quarks in the initial state (ISR) and in the final state (FSR). PYTHIA simulates the underlying event using the multiple-parton interaction model, and uses the Lund string model for hadronisation [32]. The event generator parameters are set according to the ATLAS MC09 tune [33], and the detector response is simulated using the GEANT4 program [34]. These samples are then reconstructed with the same algorithms used for data. More details on the event generation and simulation infrastructure are provided in Ref. [35]. For the study of systematic uncertainties related to the choice of the event generator and the parton-shower model, alternative samples are also generated with HERWIG 6.5 [36]. This generator also uses LO pQCD matrix elements, but has a different
parton-shower model (angle-ordered instead of $p_{\mathrm{T}}$-ordered), a different hadronisation model (the cluster model) and a different underlying event model, which is generated using the JIMMY package [37] with multipleparton interactions enabled. The HERWIG event generation parameters are also set according to the MC09 tune.

To study the main background processes, simulated samples of all relevant $2 \rightarrow 2 \mathrm{QCD}$ hard subprocesses involving only partons are used. The prompt photon contribution arising from initial and final state radiation emitted off quarks is removed from these samples in studies of the background.

Two different simulated samples are employed to study the properties of the prompt photon signal. The first sample consists of leading-order $\gamma$-jet events, and contains primarily direct photons produced in the hard subprocesses $q g \rightarrow q \gamma$ and $q \bar{q} \rightarrow g \gamma$. The second signal sample includes ISR and FSR photons emitted off quarks in all $2 \rightarrow 2$ QCD processes involving only quarks and gluons in the hard scatter. This sample is used to study the contribution to the prompt photon signal by photons from fragmentation, or from radiative corrections to the direct process, that are less isolated than those from the LO direct processes.

Finally, a sample of $W \rightarrow e \nu$ simulated events is used for the efficiency and purity studies involving electrons from $W$ decays.

## IV. THEORETICAL PREDICTIONS

The expected isolated prompt photon production cross section as a function of the photon transverse energy $E_{\mathrm{T}}^{\gamma}$ is calculated with the JETPHOX Monte Carlo program [11], which implements a full NLO QCD calculation of both the direct and the fragmentation contributions to the total cross section. In the calculation performed for this measurement, the total transverse energy carried by the partons inside a cone of radius $R=0.4$ in the $\eta-\phi$ space around the photon direction is required to be less than 4 GeV . The NLO photon fragmentation function [38] and the CTEQ 6.6 parton density functions [39] provided by the LHAPDF package [40] are used. The nominal renormalization $\left(\mu_{R}\right)$, factorization $\left(\mu_{F}\right)$ and fragmentation $\left(\mu_{f}\right)$ scales are set to the photon transverse energy $E_{\mathrm{T}}^{\gamma}$. Varying the CTEQ PDFs within the $68 \%$ C.L. intervals causes the cross section to vary between 5\% and $2 \%$ as $E_{\mathrm{T}}$ increases between 15 and 100 GeV . The variation of the three scales independently between 0.5 and 2.0 times the nominal scale changes the predicted cross section by $20 \%$ at low $E_{\mathrm{T}}$ and $10 \%$ at high $E_{\mathrm{T}}$, while the variation of the isolation requirement between 2 and 6 GeV changes the predicted cross section by no more than $2 \%$. The MSTW 2008 PDFs [41] are used as a cross-check of the choice of PDF. The central values obtained with the MSTW 2008 PDFs are between $3 \%$ and $5 \%$ higher than those predicted using the CTEQ 6.6 PDFs.

The NLO calculation provided by JETPHOX predicts a cross section at parton-level, which does not include effects of hadronisation nor the underlying event and pile-up (i.e. multiple proton-proton interactions in the same bunch crossing). The nonperturbative effects on the cross section due to hadronisation are evaluated using the simulated PYTHIA and HERWIG signal samples described in Sec. III B, by evaluating the ratio of the cross section before and after hadronisation and underlying event simulation. The ratios are estimated to be within $1 \%$ (2\%) of unity in PYTHIA (HERWIG) for all $E_{\mathrm{T}}$ and $\eta$ regions under study. To account for the effect of the underlying event and pile-up on the measured isolation energy, a correction to the photon transverse isolation energy measured in data is applied, using a procedure described in Sec. V C.

## V. PHOTON RECONSTRUCTION, IDENTIFICATION AND ISOLATION

## A. Photon reconstruction and preselection

Photon reconstruction is seeded by clusters in the electromagnetic calorimeter with transverse energies exceeding 2.5 GeV , measured in projective towers of $3 \times 5$ cells in $\eta \times \phi$ in the second layer of the calorimeter. An attempt is made to match these clusters with tracks that are reconstructed in the inner detector and extrapolated to the calorimeter. Clusters without matching tracks are directly classified as "unconverted" photon candidates. Clusters with matched tracks are considered as electron candidates. To recover photon conversions, clusters matched to pairs of tracks originating from reconstructed conversion vertices in the inner detector are considered as "converted" photon candidates. To increase the reconstruction efficiency of converted photons, conversion candidates where only one of the two tracks is reconstructed (and does not have any hit in the innermost layer of the pixel detector) are also retained $[27,28]$.

The final energy measurement, for both converted and unconverted photons, is made using only the calorimeter, with a cluster size that depends on the photon classification. In the barrel, a cluster corresponding to $3 \times 5(\eta \times \phi)$ cells in the second layer is used for unconverted photons, while a cluster of $3 \times 7(\eta \times \phi)$ cells is used for converted photon candidates (to compensate for the opening between the conversion products in the $\phi$ direction due to the magnetic field). In the end-cap, a cluster size of $5 \times 5$ is used for all candidates. A dedicated energy calibration [27] is then applied separately for converted and unconverted photon candidates to account for upstream energy loss and both lateral and longitudinal leakage.

Photon candidates with calibrated transverse energies $\left(E_{\mathrm{T}}^{\gamma}\right)$ above 15 GeV are retained for the successive analysis steps. To minimize the systematic uncertainties related to the efficiency measurement at this early stage of the experiment, the cluster barycenter in the second layer of the electromagnetic calorimeter is required to lie in
the pseudorapidity region $\left|\eta^{\gamma}\right|<1.37$, or $1.52 \leq\left|\eta^{\gamma}\right|<$ 1.81. Photon candidates with clusters containing cells overlapping with few problematic regions of the calorimeter readout are removed. After the above preselection, $1.3 \times 10^{6}$ photon candidates remain in the data sample.

## B. Photon identification

Shape variables computed from the lateral and longitudinal energy profiles of the shower in the calorimeters are used to discriminate signal from background $[27,42]$. The exact definitions of the discriminating variables are provided in Appendix A. Two sets of selection criteria (denoted "loose" and "tight") are defined, each based on independent requirements on several shape variables. The selection criteria do not depend on the photon candidate transverse energy, but vary as a function of the photon reconstructed pseudorapidity, to take into account variations in the total thickness of the upstream material and in the calorimeter geometry.

## 1. Loose identification criteria

A set of loose identification criteria for photons is defined based on independent requirements on three quantities:
(i) the leakage $R_{\text {had }}$ in the first layer of the hadronic compartment beyond the electromagnetic cluster, defined as the ratio between the transverse energy deposited in the first layer of the hadronic calorimeter and the transverse energy of the photon candidate;
(ii) the ratio $R_{\eta}$ between the energy deposits in $3 \times 7$ and $7 \times 7$ cells in the second layer of the electromagnetic calorimeter;
(iii) the root mean square (RMS) width $w_{2}$ of the energy distribution along $\eta$ in the second layer of the electromagnetic calorimeter.

True prompt photons are expected to have small hadronic leakage (typically below $1 \%-2 \%$ ) and a narrower energy profile in the electromagnetic calorimeter, more concentrated in the core of the cluster, with respect to background photon candidates from jets.

The loose identification criteria on $R_{\text {had }}, R_{\eta}$ and $w_{2}$ are identical for converted and unconverted candidates. They have been chosen, using simulated prompt photon events, in order to obtain a prompt photon efficiency, with respect to reconstruction, rising from $97 \%$ at $E_{\mathrm{T}}^{\gamma}=20 \mathrm{GeV}$ to above $99 \%$ for $E_{\mathrm{T}}^{\gamma}>40 \mathrm{GeV}$ for both converted and unconverted photons [28]. The number of photon candidates in data passing the preselection and loose photon identification criteria is $0.8 \times 10^{6}$.

## 2. Tight identification criteria

To further reject the background, the selection requirements on the quantities used in the loose identification are
tightened. In addition, the transverse shape along the $\phi$ direction in the second layer (the variable $R_{\phi}$, computed from the ratio between the energy deposits in $3 \times 3$ and $3 \times 7$ cells) and the shower shapes in the first layer of the calorimeter are examined. Several variables that discriminate single-photon showers from overlapping nearby showers (in particular those which originate from neutral meson decays to photon pairs) are computed from the energy deposited in the first layer:
(i) the total RMS width $w_{s, \text { tot }}$ of the energy distribution along $\eta$;
(ii) the asymmetry $E_{\text {ratio }}$ between the first and second maxima in the energy profile along $\eta$;
(iii) the energy difference $\Delta E$ between the second maximum and the minimum between the two maxima;
(iv) the fraction $F_{\text {side }}$ of the energy in seven strips centered (in $\eta$ ) around the first maximum that is not contained in the three core strips;
(v) the RMS width $w_{s, 3}$ of the energy distribution computed with the three core strips.
The first variable rejects candidates with wide showers consistent with jets. The second and third variables provide rejection against cases where two showers give separated energy maxima in the first layer. The last two variables provide rejection against cases where two showers are merged in a wider maximum.

The tight selection criteria are optimized independently for unconverted and converted photons to account for the quite different developments of the showers in each case. They have been determined using samples of simulated signal and background events prior to data-taking, aiming to obtain an average efficiency of $85 \%$ with respect to reconstruction for true prompt photons with transverse energies greater than 20 GeV [28]. About $0.2 \times 10^{6}$ photon candidates are retained in the data sample after applying the tight identification requirements.

## C. Photon transverse isolation energy

An experimental isolation requirement, based on the transverse energy deposited in the calorimeters in a cone around the photon candidate, is used in this measurement to identify isolated prompt photons and to further suppress the main background from $\pi^{0}$ (or other neutral hadrons decaying in two photons), where the $\pi^{0}$ is unlikely to carry the full original jet energy. The transverse isolation energy $\left(E_{\mathrm{T}}^{\mathrm{iso}}\right)$ is computed using calorimeter cells from both the electromagnetic and hadronic calorimeters, in a cone of radius 0.4 in the $\eta-\phi$ space around the photon candidate. The contributions from $5 \times 7$ electromagnetic calorimeter cells in the $\eta-\phi$ space around the photon barycenter are not included in the sum. The mean value of the small leakage of the photon energy outside this region, evaluated as a function of the photon transverse energy, is subtracted from the measured value of $E_{\mathrm{T}}^{\text {iso }}$. The typical size of this
correction is a few percent of the photon transverse energy. After this correction, $E_{\mathrm{T}}^{\text {iso }}$ for truly isolated photons is nominally independent of the photon transverse energy.

In order to make the measurement of $E_{\mathrm{T}}^{\text {iso }}$ directly comparable to parton-level theoretical predictions, such as those described in Sec. IV, $E_{\mathrm{T}}^{\text {iso }}$ is further corrected by subtracting the estimated contributions from the underlying event and from pile-up. This correction is computed on an event-by-event basis using a method suggested in Refs. [43,44]. Based on the standard seeds for jet reconstruction, which are noise-suppressed three-dimensional topological clusters [26], and for two different pseudorapidity regions ( $|\eta|<1.5$ and $1.5<|\eta|<3.0$ ), a $k_{\mathrm{T}}$ jetfinding algorithm [45,46], implemented in FASTJET [47], is used to reconstruct all jets without any explicit transverse momentum threshold. During reconstruction, each jet is assigned an area via a Voronoi tessellation [48] of the $\eta-\phi$ space. According to the algorithm, every point within a jet's assigned area is closer to the axis of that jet than of any other jet. The transverse energy density for each jet is then computed from the ratio between the jet transverse energy and its area. The ambient-transverseenergy density for the event, from pile-up and underlying event, is taken to be the median jet transverse energy density. Finally, this ambient-transverse-energy density is multiplied by the area of the isolation cone to compute the correction to $E_{\mathrm{T}}^{\text {iso }}$.

The estimated ambient-transverse-energy fluctuates significantly event-by-event, reflecting the fluctuations in the underlying event and pile-up activity in the data. The mean correction to the calorimeter transverse energy in a cone of radius $R=0.4$ for an event with one $p p$ interaction is around 440 MeV in events simulated with PYTHIA and 550 MeV in HERWIG. In the data, the mean correction is 540 MeV for events containing at least one photon candidate with $E_{\mathrm{T}}>15 \mathrm{GeV}$ and exactly one reconstructed primary vertex, and increases by an average of 170 MeV with each additional reconstructed primary vertex. The average number of reconstructed primary vertices for the sample under study is 1.56 . The distribution of measured ambient-transverse-energy densities for photons passing the tight selection criteria is shown in Fig. 1. The impact of this correction on the measured cross section is discussed in Sec. IX B. For a consistent comparison of this measurement to a theoretical prediction which incorporates an underlying event model, the method described above should be applied to the generated final state in order to evaluate and apply the appropriate event-by-event corrections.

After the leakage and ambient-transverse-energy corrections, the $E_{\mathrm{T}}^{\text {iso }}$ distribution for direct photons in simulated events is centered at zero, with an RMS width of around 1.5 GeV (which is dominated by electronic noise in the calorimeter). In the following, all photon candidates with $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$ are considered to be experimentally isolated.


FIG. 1. The measured ambient-transverse-energy densities, using the jet-area method, for events with at least one tight photon. The ambient-transverse-energy contains contributions from both the underlying event and pile-up. The broad distribution reflects the large event-to-event fluctuations.

This criterion can be related to a cut on the transverse isolation energy calculated at the parton-level in PYTHIA, in order to mimic the isolation criterion implemented in JETPHOX. This parton-level isolation is the total transverse energy of all partons that lie inside a cone of radius $R=0.4$ around the photon direction and originated from the same quark emitting the photon in either ISR or FSR. The efficiency of the experimental isolation cut at 3 GeV for photons radiated off partons in PYTHIA is close to the efficiency of a parton-level isolation cut at 4 GeV . This cut on the parton-level isolation is equivalent to the same cut on a particle-level isolation, which measures the transverse energy in a cone of radius $R=0.4$ around the photon after hadronisation (with the underlying event removed). The experimental isolation criterion is expected to reject roughly $50 \%$ of background candidates with transverse energy greater than 15 GeV .


FIG. 2. Transverse energy distribution of photon candidates selected in data, after reconstruction and preselection (open triangles) and after requiring tight identification criteria and transverse isolation energy lower than 3 GeV (full circles). The photon candidates have pseudorapidity $\left|\eta^{\gamma}\right|<1.37$ or $1.52 \leq\left|\eta^{\gamma}\right|<1.81$.

The number of photon candidates satisfying the tight identification criteria and having $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$ is 110442 : 73614 are reconstructed as unconverted photons and 36828 as converted photons. The transverse energy distribution of these candidates is shown in Fig. 2. For comparison, the initial distribution of all photon candidates after the reconstruction and preselection is also shown.

## VI. SIGNAL EFFICIENCY

## A. Reconstruction and preselection efficiency

The reconstruction and preselection efficiency, $\varepsilon_{\text {reco }}$, is computed from simulated events as a function of the true photon transverse energy for each pseudorapidity interval under study. It is defined as the ratio between the number of true prompt photons that are reconstructed-after prese-lection-in a certain pseudorapidity interval and have reconstructed $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$, and the number of true photons with true pseudorapidity in the same pseudorapidity interval and with particle-level transverse isolation energy lower than 4 GeV . The efficiency of the requirement $E_{\mathrm{T}}^{\gamma}>15 \mathrm{GeV}$ for prompt photons of true transverse energy greater than the same threshold is taken into account in Sec. VIII.

The reconstruction and preselection efficiencies are calculated using a cross-section-weighted mixture of direct photons produced in simulated $\gamma$-jet events and of fragmentation photons produced in simulated dijet events. The uncertainty on the reconstruction efficiency due to the difference between the efficiency for direct and fragmentation photons, and the unknown ratio of the two in the final sample of selected signal photons, are taken into account as sources of systematic uncertainty in Sec. IX A.

The average reconstruction and preselection efficiency for isolated prompt photons with $\left|\eta_{\text {true }}^{\gamma}\right|<1.37$ or $1.52 \leq$ $\left|\eta_{\text {true }}^{\gamma}\right|<1.81$ is around $82 \%$; the $18 \%$ inefficiency is due to the inefficiency of the reconstruction algorithms at low photon transverse energy (a few \%), to the inefficiency of the isolation requirement ( $5 \%$ ) and to the acceptance loss from a few inoperative optical links of the calorimeter readout [49].

## B. Identification efficiency

The photon identification efficiency, $\varepsilon_{\mathrm{ID}}$, is similarly computed as a function of transverse energy in each pseudorapidity region. It is defined as the efficiency for reconstructed (true) prompt photons, with measured $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$, to pass the tight photon identification criteria described in Sec. VB. The identification efficiency is determined from simulation after shifting the photon shower shapes by "shower-shape correction factors" that account for the observed average differences between the discriminating variables' distributions in data and MC. The simulated sample used contains all the main QCD signal and background processes. The average differences


FIG. 3 (color online). Efficiency of the tight identification criteria as a function of the reconstructed photon transverse energy for prompt isolated photons. Systematic uncertainties are included.
between data and simulation are computed after applying the tight identification criteria. The typical size of the correction factors is $10 \%$ of the RMS of the distribution of the corresponding variable in data, with a maximum of $50 \%$ of the RMS for the variable $\left(R_{\eta}\right)$ where the simulation is in worse agreement with the data. The corresponding correction to the MC efficiency is typically around $-3 \%$ and is always between $-5 \%$ and zero. The photon identification efficiency after all selection criteria (including isolation) are applied is shown in Fig. 3 and in Table I, including the systematic uncertainties that are discussed in more detail in Sec. IX A. The efficiencies for converted photons are, on average, $3 \%-4 \%$ lower than for unconverted photons with the same pseudorapidity and transverse energy.

As a cross-check, photon identification efficiencies are also inferred from the efficiencies of the same identification criteria applied to electrons selected in data from $W$
decays. Events containing $W \rightarrow e \nu$ candidates are selected by requiring: a missing transverse energy greater than 25 GeV (corresponding to the undetected neutrino); an opening azimuthal angle larger than 2.5 radians between the missing transverse energy vector and any energetic jets ( $E_{\mathrm{T}}>15 \mathrm{GeV}$ ) in the event; an electron transverse isolation energy in a cone of radius 0.4 in the $\eta-\phi$ space smaller than 0.3 times the electron transverse momentum; and a track, associated to the electron, that passes trackquality cuts, such as the minimum requirement on the measured transition-radiation in the transition-radiation tracker and the requirement of the presence of hits in the silicon trackers. These selection criteria, which do not rely on the shape of the electron shower in the calorimeter, are sufficient to select a $W \rightarrow e \nu$ sample with a purity (measured using a calorimeter isolation technique similar to that described in Sec. 6.1 of Ref. [50]) greater than $95 \%$. The identification efficiency of converted photons is taken from the efficiency for selected electrons to pass the tight photon selection criteria. This approximation is expected to hold to within $3 \%$ from studies of simulated samples of converted isolated prompt photons and of isolated electrons from $W$ decays. For unconverted photons, the electrons in data are used to infer shower-shape corrections. These corrections are then applied to unconverted photons in simulation, in order to calculate the unconverted photon efficiency from Monte Carlo. The results from the electron extrapolation method are consistent with those from the simulation, with worse precision due to the limited statistics of the selected electron sample.

## C. Trigger efficiency

The efficiency of the calorimeter trigger, relative to the photon reconstruction and identification selection, is defined as the probability for a true prompt photon, passing the tight photon identification criteria and with $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$, to pass the trigger selection. It is estimated in two steps. First, using a prescaled sample of minimum-bias triggers, the efficiency of a lower threshold ( $\approx 3.5 \mathrm{GeV}$ ) level-1 calorimeter trigger is determined. The measured efficiency of this trigger is $100 \%$ for all photon

TABLE I. Isolated prompt photon identification efficiency in the intervals of the photon pseudorapidity and transverse energy under study.

| $E_{\mathrm{T}}^{\gamma}[\mathrm{GeV}]$ | $0.00 \leq\left\|\eta^{\gamma}\right\|<0.60$ | Identification Efficiency $[\%]$ <br> $0.60 \leq\left\|\eta^{\gamma}\right\|<1.37$ | $1.52 \leq\left\|\eta^{\gamma}\right\|<1.81$ |
| :--- | :---: | :---: | :---: |
| $[15,20)$ | $63.3 \pm 6.6$ | $63.5 \pm 6.9$ | $72.2 \pm 8.4$ |
| $[20,25)$ | $73.5 \pm 6.1$ | $73.5 \pm 6.8$ | $81.6 \pm 8.3$ |
| $[25,30)$ | $80.2 \pm 5.4$ | $80.8 \pm 5.7$ | $86.7 \pm 6.6$ |
| $[30,35)$ | $85.5 \pm 4.5$ | $85.3 \pm 4.8$ | $90.4 \pm 5.9$ |
| $[35,40)$ | $85.2 \pm 3.9$ | $89.3 \pm 4.3$ | $92.3 \pm 5.0$ |
| $[40,50)$ | $89.2 \pm 3.3$ | $92.1 \pm 3.6$ | $93.5 \pm 4.6$ |
| $[50,60)$ | $91.3 \pm 3.1$ | $94.1 \pm 2.8$ | $93.9 \pm 3.6$ |
| $[60,100)$ | $92.2 \pm 2.6$ | $94.8 \pm 2.6$ | $94.2 \pm 2.9$ |



FIG. 4. Photon trigger efficiency, with respect to reconstructed isolated photon passing the tight identification criteria, as measured in data (circles) and simulated background events (triangles).
candidates with reconstructed $E_{\mathrm{T}}^{\gamma}>15 \mathrm{GeV}$ passing tight identification criteria. Then, the efficiency of the high-level trigger is measured using the sample of events that pass the level-1 calorimeter trigger with the 3.5 GeV threshold.

The trigger efficiency for reconstructed photon candidates passing tight selection criteria, isolated and with $E_{\mathrm{T}}^{\gamma}>15 \mathrm{GeV}$ is found to be $\varepsilon^{\text {trig }}=(99.5 \pm 0.5) \%$, constant within uncertainties over the full $E_{\mathrm{T}}$ and $\eta$ ranges under study. The quoted uncertainty is obtained from the estimation of the possible bias introduced by using photon candidates from data, which are a mixture of signal and background photon candidates. Using Monte Carlo samples the absolute difference of the trigger efficiency for a pure signal sample and for a pure background sample is found to be smaller than $0.5 \%$ for isolated tight photon candidates with $E_{\mathrm{T}}^{\gamma}>15 \mathrm{GeV}$.

A comparison between the high-level trigger efficiency in data and in the background predicted by the simulation is shown in Fig. 4.

## VII. BACKGROUND SUBTRACTION AND SIGNAL YIELD DETERMINATION

A non-negligible residual contribution of background candidates is expected in the selected photon sample, even after the application of the tight identification and isolation requirements. Two methods are used to estimate the background contribution from data and to measure the prompt photon signal yield. The first one is used for the final cross section measurement, while the second one is used as a cross-check of the former. All estimates are made separately for each region of pseudorapidity and transverse energy.

## A. Isolation vs identification sideband counting method

The first technique for measuring the prompt photon yield uses the number of photon candidates observed in the sidebands of a two-dimensional distribution to estimate
the amount of background in the signal region. The two dimensions are defined by the transverse isolation energy $E_{\mathrm{T}}^{\text {iso }}$ on one axis, and the photon identification $\left(\gamma_{\mathrm{ID}}\right)$ of the photon candidate on the other axis. On the isolation axis, the signal region contains photon candidates with $E_{\mathrm{T}}^{\mathrm{iso}}<3 \mathrm{GeV}$, while the sideband contains photon candidates with $E_{\mathrm{T}}^{\mathrm{iso}}>5 \mathrm{GeV}$. On the other axis, photon candidates passing the tight identification criteria (tight candidates) belong to the $\gamma_{\mathrm{ID}}$ signal region, while those that fail the tight identification criteria but pass a background-enriching selection ("nontight" candidates) belong to the $\gamma_{\mathrm{ID}}$ sideband. The nontight selection requires photon candidates to fail at least one of a subset of the photon tight identification criteria, but to pass all criteria not in that subset. All the shower-shape variables based on the energy measurement in the first layer of the electromagnetic calorimeter are used to define the backgroundenriching selection, with the exception of $w_{s, \text { tot }}$, since it is found to be significantly correlated with the $E_{\mathrm{T}}^{\text {iso }}$ of background photon candidates, while the photon yield measurement relies on the assumption of negligible (or small) correlations between the transverse isolation energy and the shower-shape quantities used to define the backgroundenriching selection.

The signal region (region " $A$ ") is therefore defined by photon candidates passing the tight photon identification criteria and having experimental $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$. The three background control regions consist of photon candidates either:
(i) passing the tight photon identification criteria but having experimental $E_{\mathrm{T}}^{\text {iso }}>5 \mathrm{GeV}$ (region " B ")
(ii) having $E_{\mathrm{T}}^{\mathrm{iso}}<3 \mathrm{GeV}$ and passing the backgroundenriching identification criteria (region "C")
(iii) having $E_{\mathrm{T}}^{\text {iso }}>5 \mathrm{GeV}$ and passing the backgroundenriching identification criteria (region " $D$ ").

A sketch of the two-dimensional plane and of the signal and background control region definitions is shown in Fig. 5.

The method assumes that the signal contamination in the three background control regions is small, and that the isolation profile in the nontight regions is the same as that of the background in the tight regions. If these assumptions hold, then the number of background candidates in the signal region can be calculated by taking the ratio of candidates in the two nontight regions $\left(N_{C} / N_{D}\right)$, and multiplying it by the number of candidates in the tight, nonisolated region $\left(N_{B}\right)$. The number of isolated prompt photons passing the tight identification criteria is therefore:

$$
\begin{equation*}
N_{A}^{\text {sig }}=N_{A}-N_{B} \frac{N_{C}}{N_{D}}, \tag{1}
\end{equation*}
$$

where $N_{A}$ is the observed number of photon candidates in the signal region.


FIG. 5 (color online). Illustration of the two-dimensional plane, defined by means of the transverse isolation energy and a subset of the photon identification (ID) variables, used for estimating, from the observed yields in the three control regions $(B, C, D)$, the background yield in the signal region $(A)$.

The assumption that the signal contamination in the background control regions is small is checked using prompt photon MC samples. As the number of signal events in the background control regions is always positive and nonzero, corrections are applied to limit the effects on the final result. For this purpose, Eq. (1) is modified in the following way:

$$
\begin{equation*}
N_{A}^{\mathrm{sig}}=N_{A}-\left(N_{B}-c_{B} N_{A}^{\mathrm{sig}}\right) \frac{\left(N_{C}-c_{C} N_{A}^{\mathrm{sig}}\right)}{\left(N_{D}-c_{D} N_{A}^{\mathrm{sig}}\right)}, \tag{2}
\end{equation*}
$$

where $c_{K} \equiv \frac{N_{K}^{\text {it }}}{N_{A}^{\mathrm{E}_{8}}}($ for $K \in\{B, C, D\})$ are the signal leakage fractions extracted from simulation. Typical values for $c_{B}$ are between $3 \%$ and $17 \%$, increasing with the photon candidate transverse energy; for $c_{C}$, between $2 \%$ and $14 \%$, decreasing with $E_{\mathrm{T}}^{\gamma}$. $c_{D}$ is always less than $2 \%$. The total effect of these corrections on the measured signal photon purities is typically less than $5 \%$.

The isolated prompt photon fraction measured with this method, as a function of the photon reconstructed


FIG. 6 (color online). Fraction of isolated prompt photons as a function of the photon transverse energy, as obtained with the two-dimensional sideband method.
transverse energy, is shown in Fig. 6. The numbers of isolated prompt photon candidates measured in each pseudorapidity and transverse energy interval are also reported in Table II. The systematic uncertainties on the measured prompt photon yield and fraction in the selected sample are described in Sec. IX B.

## B. Isolation template fit method

The second method relies on a binned maximum likelihood fit to the $E_{\mathrm{T}}^{\mathrm{iso}}$ distribution of photon candidates selected in data which pass the tight identification criteria. The distribution is fit to the sum of a signal template and a background template, determined from control samples extracted from data. This is similar to the technique employed in [20], but relies less on simulation for signal and background templates. The signal template is determined from the $E_{\mathrm{T}}^{\text {iso }}$ distribution of electrons from $W$ and $Z$

TABLE II. Observed number of isolated prompt photons in the photon transverse energy and pseudorapidity intervals under study. The first uncertainty is statistical, the second is the systematic uncertainty, evaluated as described in Sec. IX B.

|  | Isolated prompt photon yield |  |  |
| :--- | :---: | :---: | :---: |
| $E_{\mathrm{T}}^{\gamma}[\mathrm{GeV}]$ | $0.00 \leq\left\|\eta^{\gamma}\right\|<0.60$ | $0.60 \leq\left\|\eta^{\gamma}\right\|<1.37$ | $1.52 \leq\left\|\eta^{\gamma}\right\|<1.81$ |
| $[15,20)$ | $\left(119 \pm 3_{-20}^{+12}\right) \times 10^{2}$ | $\left(130 \pm 4_{-11}^{+40}\right) \times 10^{2}$ | $\left(72 \pm 2_{-7}^{+20}\right) \times 10^{2}$ |
| $[20,25)$ | $\left(501 \pm 12_{-53}^{+47}\right) \times 10^{1}$ | $\left(578 \pm 18_{-45}^{+125}\right) \times 10^{1}$ | $\left(304 \pm 10_{-23}^{+40}\right) \times 10^{1}$ |
| $[25,30)$ | $\left(260 \pm 7_{-21}^{+20}\right) \times 10^{1}$ | $\left(306 \pm 10_{-18}^{+46}\right) \times 10^{1}$ | $\left(135 \pm 6_{-10}^{+16}\right) \times 10^{1}$ |
| $[30,35)$ | $\left(146 \pm 5_{-6}^{+9}\right) \times 10^{1}$ | $\left(160 \pm 6_{-9}^{+19}\right) \times 10^{1}$ | $\left(73 \pm 4_{-5}^{+8}\right) \times 10^{1}$ |
| $[35,40)$ | $\left(82 \pm 4_{-4}^{+5}\right) \times 10^{1}$ | $\left(102 \pm 4_{-6}^{+9}\right) \times 10^{1}$ | $\left(44 \pm 3_{-3}^{+5}\right) \times 10^{1}$ |
| $[40,50)$ | $\left(77 \pm 3_{-4}^{+5}\right) \times 10^{1}$ | $\left(98 \pm 4_{-7}^{+9}\right) \times 10^{1}$ | $\left(38 \pm 2_{-2}^{+3}\right) \times 10^{1}$ |
| $[50,60)$ | $\left(329 \pm 20_{-14}^{+17}\right) \times 10^{0}$ | $(420 \pm 20 \pm 30) \times 10^{0}$ | $\left(147 \pm 16_{-17}^{+16}\right) \times 10^{0}$ |
| $[60,100)$ | $\left(329 \pm 20_{-15}^{+19}\right) \times 10^{0}$ | $\left(370 \pm 20_{-20}^{+30}\right) \times 10^{0}$ | $\left(154 \pm 12_{-8}^{+12}\right) \times 10^{0}$ |

decays, selected using the criteria described in [50]. Electrons from $W$ decays are required to fulfill tight selection criteria on the shapes of their showers in the electromagnetic calorimeter and to pass track-quality requirements, including the presence of transition-radiation hits. They must also be accompanied by $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$, and the electron- $E_{\mathrm{T}}^{\text {miss }}$ system must have a transverse mass larger than 40 GeV . Electrons from $Z$ decays are selected with looser criteria, but the pair must have an invariant mass close to the $Z$ mass. A single signal template is constructed for each region in $|\eta|$, exploiting the independence of $E_{\mathrm{T}}^{\text {iso }}$ from the transverse energy of the object (after applying the corrections described in Sec. V C) to maximize the available statistics. A small bias is expected due to differences between the electron and photon $E_{\mathrm{T}}^{\text {iso }}$ distributions, especially in regions where there is significant material upstream of the calorimeter. A shift of the signal template is applied to the electron distributions extracted from data to compensate for the differences between electrons and photons seen in simulation. This shift, computed using simulated photon and electron samples, increases from 100 MeV to 600 MeV with increasing $\left|\eta^{\gamma}\right|$. The background template is extracted from data for each $\left(E_{\mathrm{T}},|\eta|\right)$ bin, using the same reverse-cuts procedure as in the two-dimensional sideband technique. A simulationbased correction, typically of the order of $3 \%-4 \%$, is applied to the final photon fraction to account for a signal which leaks into the background template. The fit is performed in each region of $\left|\eta^{\gamma}\right|$ for the individual bins in transverse energy, and the signal yield and fraction are extracted. An example of such a fit is shown in Fig. 7. The results from this alternative technique are in good agreement with those from the simpler counting method described in the previous subsection, with differences


FIG. 7 (color online). Example of a fit to extract the fraction of prompt photons using the isolation template technique in the region $0 \leq|\eta|<0.6$ and $35 \leq E_{\mathrm{T}}^{\gamma}<40 \mathrm{GeV}$. The signal template is derived from electrons selected from $W$ or $Z$ decays, and is shown with a dashed line. The background template is derived from a background-enriched sample, and is represented by a dotted line. The estimated photon fraction is 0.85 and its statistical uncertainty is 0.01 .
typically smaller than $2 \%$ and within the systematic uncertainties that are uncorrelated between the two methods.

## C. Electron background subtraction

The background of prompt electrons misidentified as photons needs also to be considered. The dominant electron production mechanisms are semileptonic hadron decays (mostly from hadrons containing heavy flavor quarks) and decays of electroweak bosons (the largest contribution being from $W$ decays). Electrons from the former are often produced in association with jets, and have $E_{\mathrm{T}}^{\text {iso }}$ profiles similar to the dominant backgrounds from light mesons. They are therefore taken into account and subtracted using the two-dimensional sideband technique described in Sec. VII A. Conversely, electrons from $W$ and $Z$ decays have $E_{\mathrm{T}}^{\mathrm{iso}}$ profiles that are similar to those of signal photons. The contribution of this background to the signal yield computed in Sec. VII A needs therefore to be removed before the final measurement of the cross section.

The fraction of electrons reconstructed as photon candidates is estimated from the data, as a function of the electron transverse energy and pseudorapidity, using a control sample of $Z \rightarrow e^{+} e^{-}$decays. The average electron misidentification probability is around $8 \%$. Using the $W \rightarrow e \nu$ and $Z \rightarrow e e$ cross section times branching ratio measured by ATLAS in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ [50], the estimated fraction of photon candidates due to isolated electrons is found to be on average $\sim 0.5 \%$, varying significantly with transverse energy. A maximum contamination of $(2.5 \% \pm 0.8 \%)$ is estimated for transverse energies between 40 and 50 GeV , due to the kinematic distribution of electrons from $W$ and $Z$ decays. The uncertainties on these estimates are less than $1 \%$ of the photon yield.

## VIII. CROSS SECTION MEASUREMENT

The differential cross section is measured by computing:

$$
\begin{equation*}
\frac{d \sigma}{d E_{\mathrm{T}}^{\gamma}}=\frac{N_{\text {yield }} U}{\left(\int \mathcal{L} d t\right) \Delta E_{\mathrm{T}}^{\gamma} \varepsilon_{\text {trigger }} \varepsilon_{\mathrm{reco}} \varepsilon_{\mathrm{ID}}} \tag{3}
\end{equation*}
$$

The observed signal yield ( $N_{\text {yield }}$ ) is divided by the widths of the $E_{\mathrm{T}}$-intervals $\left(\Delta E_{\mathrm{T}}^{\gamma}\right)$ and by the product of the photon identification efficiency ( $\varepsilon_{\mathrm{ID}}$, determined in Sec. VIB) and of the trigger efficiency relative to photon candidates passing the identification criteria ( $\varepsilon_{\text {trigger }}$, determined in Sec. VIC). The spectrum obtained this way, which depends on the reconstructed transverse energy of the photon candidates, is then corrected for detector energy resolution and energy scale effects using bin-by-bin correction factors (the "unfolding coefficients" $U$ ) evaluated using simulated samples. The corrected spectrum, which is then a function of the true photon energy, is divided by the photon reconstruction efficiency $\varepsilon_{\text {reco }}$ (Sec. VI A) and by the integrated luminosity of the data sample, $\int \mathcal{L} d t$.

The unfolding coefficients are evaluated from the ratio of the true to reconstructed $E_{\mathrm{T}}$ distributions of photon candidates, using PYTHIA isolated prompt photon simulated samples. This procedure is justified by the small bin-to-bin migrations (typically of the order of a few \%) that are expected, given the good electromagnetic calorimeter energy resolution compared to the width of the transverse energy intervals used in this analysis (between 5 and 40 GeV ). The values of the unfolding coefficients are slightly higher than 1 and decrease as a function of $E_{\mathrm{T}}$, approaching 1 . They differ from 1 by less then $2 \%$ in the $\left|\eta^{\gamma}\right|$ region between 0.0 and 0.6 , and by less than $5 \%-7 \%$ in the other two $\left|\eta^{\gamma}\right|$ regions, where more material upstream of the electromagnetic calorimeter is present.

## IX. SYSTEMATIC UNCERTAINTIES

Several sources of systematic uncertainties on the cross section are identified and evaluated as described in the following sections. The total systematic uncertainty is obtained by combining the various contributions, taking into account their correlations: uncorrelated uncertainties are summed in quadrature while a linear sum of correlated uncertainties is performed.

## A. Reconstruction, identification, trigger efficiencies

The systematic uncertainty on the reconstruction efficiency from the experimental isolation requirement is evaluated from the prompt photon simulation varying the value of the isolation criterion by the average difference (of the order of 500 MeV ) observed for electrons from $W$ and $Z$ decays in simulation and data. It is $2.5 \%$ in the pseudorapidity regions covered by the barrel calorimeter and $4.5 \%$ in the end-caps.

The systematic uncertainty on the identification efficiency due to the photon shower-shape corrections is divided into two parts. The first term evaluates the impact of treating the differences between the distributions of the shower-shape variables in data and simulation as an average shift. This uncertainty is evaluated in the following way:
(i) A modified description of the detector material is used to produce a second sample of simulated photon candidates. These candidates have different showershape distributions, due to the different amount of material upstream of and within the calorimeter. This alternative model contains an additional $10 \%$ of material in the inactive volumes of the inner detector and $10 \%$ of a radiation length in front of the electromagnetic calorimeter. This model is estimated to represent a conservative upper limit of the additional detector material that is not accounted for by the nominal simulation.
(ii) The correction procedure is applied to the nominal simulation to estimate the differences between the nominal and the alternative simulation. The shifts between the discriminating variable distributions in the nominal and the alternative simulation are eval-
uated, and are used to correct the shower-shape variable distributions of the nominal simulation.
(iii) The photon efficiency from the nominal simulation is recomputed after applying these corrections, and compared with the efficiency obtained from the alternative simulation.

The difference between the efficiency estimated from the nominal simulation (after applying the corrections) and the efficiency measured directly in the alternative sample (with no corrections) ranges from $3 \%$ at $E_{\mathrm{T}}^{\gamma} \sim 20 \mathrm{GeV}$ to less than $1 \%$ at $E_{\mathrm{T}}^{\gamma} \sim 80 \mathrm{GeV}$.

The second part of the systematic uncertainty on the identification efficiency accounts for the uncertainty on the extracted shower-shape correction factors. The correction factors were extracted by comparing tight photons in data and simulation; to evaluate the uncertainty associated with this choice, the same correction factors are extracted using loose photons. The difference in the final efficiency when applying the tight corrections and the loose corrections is then taken as the uncertainty. This uncertainty drops from $4 \%$ to $1 \%$ with increasing $E_{\mathrm{T}}^{\gamma}$.

Additional systematic uncertainties that may affect both the reconstruction and the identification efficiencies are evaluated simultaneously for the product of the two, to take into account possible correlations. These sources of uncertainty include the amount of material upstream of the calorimeter; the impact of pile-up; the relative fraction of direct and fragmentation photons in data with respect to simulation; the misidentification of a converted photon as unconverted; the difference between the PYTHIA and HERWIG simulation models; the impact of a sporadic faulty calibration of the cell energies in the electromagnetic calorimeter; and the imperfect simulation of acceptance losses due to inoperative readout links in the calorimeter.

Of all the uncertainties which contribute to this measurement, the largest ones come from the uncertainty on the amount of material upstream of the calorimeter (absolute uncertainties ranging between $1 \%$ and $8 \%$ and are larger at low $E_{\mathrm{T}}^{\gamma}$ ), and from the uncertainty on the identification efficiency due to the photon shower-shape corrections (the absolute uncertainties are in the range $1 \%-5 \%$, and are larger at low $E_{\mathrm{T}}^{\gamma}$ ).

The uncertainty on the trigger efficiency, evaluated as described in Sec. VIC, is $0.5 \%$ and is nearly negligible compared to all other sources.

## B. Signal yield estimates

The following sources of systematic uncertainties affecting the accuracy of the signal yield measurement using the two-dimensional sideband technique are considered.

## 1. Background isolation control region definition

The signal yield is evaluated after changing the isolation control region definition. The minimum value of $E_{\mathrm{T}}^{\text {iso }}$ re-
quired for candidates in the nonisolated control regions, which is set to 5 GeV in the nominal measurement, is changed to 4 and 6 GeV . This check is sensitive to uncertainties in the contribution of prompt photons from QED radiation from quarks: these photons are less isolated than those originating from the hard process. Alternative measurements are also performed where a maximum value of $E_{\mathrm{T}}^{\text {iso }}$ is set to 10 or 15 GeV for candidates in the nonisolated control regions, in order to reduce the correlation between the isolation variable and the shower-shape distributions seen in simulated events for candidates belonging to the upper tail of the isolation distribution. The largest positive and negative variations of the signal yield with respect to the nominal result are taken as systematic uncertainties. The signal photon fraction changes by at most $\pm 2 \%$ in all the transverse energy and pseudorapidity intervals.

## 2. Background photon identification control region definition

The measurement is repeated reversing the tight identification criteria on a number of strip variables ranging between two (only $F_{\text {side }}$ and $w_{s 3}$ ) and five (all the variables based on the first layer of the electromagnetic calorimeter). The largest positive and negative variations of the signal yield (with respect to the nominal result) from these three alternative measurements are taken as systematic uncertainties. The effect on the signal photon fraction decreases with increasing photon transverse energy, and is around $10 \%$ for $E_{\mathrm{T}}^{\gamma}$ between 15 and 20 GeV .

## 3. Signal leakage into the photon identification background control region

From the photon identification efficiency studies, an upper limit of $5 \%$ is set on the uncertainty on the fraction $c_{C}$ of signal photons passing all the tight photon identification criteria except those used to define the photon identification control region. The signal yields in each $E_{\mathrm{T}}^{\gamma},\left|\eta^{\gamma}\right|$ interval are thus measured again after varying the estimated signal contamination in the photon identification control regions ( $c_{C}$ and $c_{D} / c_{B}$ ) by this uncertainty, and the difference with the nominal result is taken as a systematic uncertainty. The signal fraction variations are always below $6 \%$.

## 4. Signal leakage into the isolation background control region

The fractions $c_{B}$ and $c_{D}$ of signal photons contaminating the isolation control regions depend on the relative amount of direct and fragmentation photons in the signal selected in a certain $E_{\mathrm{T}}^{\gamma},\left|\eta^{\gamma}\right|$ interval, since the latter are characterized by larger nearby activity, and therefore usually have slightly larger transverse isolation energies. In the nominal measurement, the values of $c_{B}$ and $c_{D}$ are computed with
the relative fractions of direct and fragmentation photons predicted by PYTHIA. A systematic uncertainty is assigned by repeating the measurement after varying these fractions between $0 \%$ and $100 \%$. The measured signal photon fraction varies by less than $5 \%$.

## 5. Signal photon simulation

The signal yield is estimated using samples of prompt photons simulated with HERWIG instead of PYTHIA to determine the fraction of signal leaking into the three background control regions. The variations of the signal photon fractions in each $E_{\mathrm{T}}^{\gamma},\left|\eta^{\gamma}\right|$ interval are below $2 \%$.

## 6. Correlations between the isolation and the photon identification variables for background candidates

Non-negligible correlations between the isolation variable and the photon identification quantities would affect Eq. (2): the true number of isolated tight prompt photon candidates would be

$$
\begin{equation*}
N_{A}^{\mathrm{sig}}=N_{A}-R^{\mathrm{bkg}}\left(N_{B}-c_{B} N_{A}^{\mathrm{sig}}\right) \frac{\left(N_{C}-c_{C} N_{A}^{\mathrm{sig}}\right)}{\left(N_{D}-c_{D} N_{A}^{\mathrm{sig}}\right)} \tag{4}
\end{equation*}
$$

where $R^{\mathrm{bkg}} \equiv \frac{N_{A}^{\mathrm{bkg}} N_{D}^{\mathrm{bkg}}}{N_{B}^{\mathrm{bg} \mathrm{g}} N_{C}^{\mathrm{bg}}}$ would then be different from unity. The simulation of background events shows a small but non-negligible correlation between the isolation and the discriminating shower-shape variables used to define the photon identification signal and background control regions. The signal yields are therefore recomputed with the formula in Eq. (4), using for $R^{\text {bkg }}$ the value predicted by the PYTHIA background simulation, and compared with the nominal results. The effect is smaller than $0.6 \%$ in the $\left|\eta^{\gamma}\right|<1.37$ intervals and around $3.6 \%$ for $1.52 \leq$ $\left|\eta^{\gamma}\right|<1.81$.

## 7. Transverse isolation energy corrections

The effects of the $E_{\mathrm{T}}^{\text {iso }}$ correction for the underlying event on the estimated signal yield are also investigated. The impact of this correction is evaluated by estimating the signal yield, with and without the correction applied, for events with only one reconstructed primary vertex (to eliminate any effects of pile-up). The estimated signal yields using the uncorrected values of $E_{\mathrm{T}}^{\text {iso }}$, normalized to the yields derived using the corrected values, show no trend in $E_{\mathrm{T}}^{\gamma}$ or $\eta$. Furthermore, the impact on the cross section of the event-by-event corrections is equivalent to that of an average correction of 540 MeV applied to the transverse isolation energies of all photon candidates. Similar studies in PYTHIA and HERWIG MC yield identical results.

## C. Unfolding coefficients

The unfolding coefficients used to correct the measured cross section for $E_{\mathrm{T}}$ bin-by-bin migrations are computed
using simulated samples. There are three sources of uncertainties on these coefficients.

## 1. Energy scale uncertainty

The uncertainty on the energy scale was estimated to be $\pm 3 \%$ in test beam studies [51], and is confirmed to be below this value from the comparison of the $Z \rightarrow e^{+} e^{-}$ invariant mass peak in data and Monte Carlo. The unfolding coefficients are thus recomputed using simulated signal events where the true photon energy is shifted by $\pm 3 \%$. The coefficients change by $\pm 10 \%$. This uncertainty introduces a relative uncertainty of about $10 \%$ on the measured cross section which is fully correlated between the different $E_{\mathrm{T}}^{\gamma}$ intervals within each pseudorapidity range.

## 2. Energy resolution uncertainty

The uncertainty on the energy resolution may affect bin-by-bin migrations between adjacent $E_{\mathrm{T}}$ bins. Test beam studies indicate that the sampling terms of the resolution in data and simulation have a relative difference within $20 \%$. Furthermore, studies of the $Z \rightarrow e^{+} e^{-}$invariant mass distribution in data indicate that the constant term of the calorimeter energy resolution is below $1.5 \%$ in the barrel and $3.0 \%$ in the end-cap (it is $0.7 \%$ in the simulation). The unfolding coefficients are thus recomputed after smearing the reconstructed energy of simulated photons to take into account a $20 \%$ relative increase of the sampling term and a constant term of $1.5 \%$ in the barrel and $3.0 \%$ in the endcap. The resulting variation of the unfolding coefficients is always less than $1 \%$. The uncertainty arising from nongaussian tails of the energy resolution function is estimated by recomputing the coefficients using a prompt photon simulation where a significant amount of material is added to the detector model. The variations of the unfolding coefficients are smaller than $1 \%$ in all the pseudorapidity and transverse energy intervals under study.

## 3. Simulated photon transverse energy distribution

The unfolding coefficients, computed in $E_{\mathrm{T}}^{\gamma}$ intervals of non-negligible size, depend on the initial $E_{\mathrm{T}}^{\gamma}$ distribution predicted by PYTHIA. An alternative unfolding technique [52] is therefore used, which relies on the repeated application of Bayes' theorem to iteratively obtain an improved estimate of the unfolded spectrum. This technique relies less on the simulated original $E_{\mathrm{T}}$ distribution of the prompt photons. The differences between the cross-sections estimated using the bin-by-bin unfolding and the iterative Bayesian unfolding are within $2 \%$, and are taken into account as an additional systematic uncertainty.

## D. Luminosity

The integrated luminosity is determined for each run by measuring interaction rates using several ATLAS subdetectors at small angles to the beam line, with the absolute
calibration obtained from beam position scans [53]. The relative systematic uncertainty on the luminosity measurement is estimated to be $11 \%$ and translates directly into an $11 \%$ relative uncertainty on the cross section.

## X. RESULTS AND DISCUSSION

The measured inclusive isolated prompt photon production cross sections $d \sigma / d E_{\mathrm{T}}^{\gamma}$ are shown in Fig. 8-10. They are presented as a function of the photon transverse energy, for each of the three considered pseudorapidity intervals. They are also presented in tabular form in Appendix B. The measurements extend from $E_{\mathrm{T}}^{\gamma}=15 \mathrm{GeV}$ to $E_{\mathrm{T}}^{\gamma}=$ 100 GeV spanning almost 3 orders of magnitude. The data are compared to NLO pQCD calculations, obtained with the JETPHOX program as described in Sec. IV. The error bars on the data points represent the combination of the statistical and systematic uncertainties (summed in quadrature): systematic uncertainties dominate over the whole considered kinematic range. The contribution from the luminosity uncertainty ( $11 \%$ ) is shown separately (dotted bands) as it represents a possible global offset of all the measurements. The total systematic uncertainties on the theoretical predictions are represented with a solid band. They are obtained by summing in quadrature the contributions from the scale uncertainty, the PDF uncertainty (at $68 \%$ C.L.) and the uncertainty associated with the choice of the parton-level isolation criterion. The same quantities are also shown, in the bottom panels of Fig. 8-10, after having been normalized to the expected NLO pQCD cross sections.

In general, the theoretical predictions agree with the measured cross sections for $E_{\mathrm{T}}^{\gamma}>25 \mathrm{GeV}$. For lower $E_{\mathrm{T}}$


FIG. 8 (color online). Measured (dots) and expected (full line) inclusive prompt photon production cross sections, as a function of the photon transverse energies above 15 GeV and in the pseudorapidity range $\left|\eta^{\gamma}\right|<0.6$. The bottom panel shows the ratio between the measurement and the theoretical prediction.


FIG. 9 (color online). Measured (dots) and expected (full line) inclusive prompt photon production cross sections, as a function of the photon transverse energies above 15 GeV and in the pseudorapidity range $0.6 \leq\left|\eta^{\gamma}\right|<1.37$. The bottom panel shows the ratio between the measurement and the theoretical prediction.
and in the two pseudorapidity regions $\left|\eta^{\gamma}\right|<0.6$ and $0.6 \leq\left|\eta^{\gamma}\right|<1.37$, the cross section predicted by JETPHOX is larger than that measured in data. Such low transverse energies at the LHC correspond to extremely small values of $x_{\mathrm{T}}=2 E_{\mathrm{T}}^{\gamma} / \sqrt{s}$, where NLO theoretical predictions are less accurate. In such a regime the appropriate values of the different scales are not clearly defined, and the uncertainties associated with these scales in the theoretical predictions may not be well modeled by simple


FIG. 10 (color online). Measured (dots) and expected (full line) inclusive prompt photon production cross sections, as a function of the photon transverse energies above 15 GeV and in the pseudorapidity range $1.52 \leq\left|\eta^{\gamma}\right|<1.81$. The bottom panel shows the ratio between the measurement and the theoretical prediction.
variations of any one scale about the default value of $E_{\mathrm{T}}^{\gamma}$ [54]. As the low- $E_{\mathrm{T}}^{\gamma}$ region is where the fragmentation component has the most significant contribution to the total cross section, the total uncertainty associated with the NLO predictions at low $E_{\mathrm{T}}^{\gamma}$ may be underestimated.

## XI. CONCLUSION

The inclusive isolated prompt photon production cross section in $p p$ collisions at a center-of-mass energy $\sqrt{s}=7 \mathrm{TeV}$ has been measured using $880 \mathrm{nb}^{-1}$ of $p p$ collision data collected by the ATLAS detector at the Large Hadron Collider.

The differential cross section has been measured as a function of the prompt photon transverse energy between 15 and 100 GeV , in the three pseudorapidity intervals $\left|\eta^{\gamma}\right|<0.6, \quad 0.6 \leq\left|\eta^{\gamma}\right|<1.37$ and $1.52 \leq\left|\eta^{\gamma}\right|<1.81$, estimating the background from the selected photon sample and using the photon identification efficiency measurement described in this paper. The photon identification using the fine granularity of the calorimeters. A photon isolation criterion is used, after an in situ subtraction of the effects of the underlying event that may also be applied to theoretical predictions.

The observed cross sections rapidly decrease as a function of the increasing photon transverse energy, spanning almost 3 orders of magnitude. The precision of the measurement is limited by its systematic uncertainty, which receives important contributions from the energy scale uncertainty, the luminosity, the photon identification efficiency, and the uncertainty on the residual background contamination in the selected photon sample.

The NLO pQCD predictions agree with the observed cross sections for transverse energies greater than 25 GeV , while for transverse energies below 25 GeV the cross sections predicted by JETPHOX are higher than measured. However, the precision of this comparison below 25 GeV is limited by large systematic uncertainties on the measurement and on the theoretical predictions at such low values of $x_{\mathrm{T}}=2 E_{\mathrm{T}}^{\gamma} / \sqrt{s}$.

The measured prompt photon production cross section is more than a factor of 30 larger than that measured at the Tevatron, and a factor of $10^{4}$ larger than for photoproduction at HERA, assuming a similar kinematic range in transverse energy and pseudorapidity. This will allow the extension of the measurement up to energies in the TeV range after only a few years of data-taking at the LHC.

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## APPENDIX A: DEFINITION OF PHOTON IDENTIFICATION DISCRIMINATING VARIABLES

In this Appendix, the quantities used in the selection of photon candidates, based on the reconstructed energy deposits in the ATLAS calorimeters, are summarized.
(1) Leakage in the hadronic calorimeter

The following discriminating variable is defined, based on the energy deposited in the hadronic calorimeter:
(a) Normalized hadronic leakage

$$
\begin{equation*}
R_{\mathrm{had}}=\frac{E_{\mathrm{T}}^{\mathrm{had}}}{E_{\mathrm{T}}} \tag{A1}
\end{equation*}
$$

is the total transverse energy $E_{\mathrm{T}}^{\text {had }}$ deposited in the hadronic calorimeter, normalized to the total transverse energy $E_{\mathrm{T}}$ of the photon candidate.

In the $|\eta|$ interval between 0.8 and 1.37 the energy deposited in the whole hadronic calorimeter is used, while in the other pseudorapidity intervals only the leakage in the first layer of the hadronic calorimeter is used.
(2) Variables using the second ("middle") layer of the electromagnetic calorimeter
The discriminating variables based on the energy deposited in the second layer of the electromagnetic calorimeter are the following:
(a) Middle $\eta$ energy ratio

$$
\begin{equation*}
R_{\eta}=\frac{E_{3 \times 7}^{S 2}}{E_{7 \times 7}^{S 2}} \tag{A2}
\end{equation*}
$$

is the ratio between the sum $E_{3 \times 7}^{S 2}$ of the energies of the second layer cells of the electromagnetic calorimeter contained in a $3 \times 7$ rectangle in $\eta \times \phi$ (measured in cell units), and the sum $E_{7 \times 7}^{S 2}$ of the energies in a $7 \times 7$ rectangle, both centered around the cluster seed.
(b) Middle $\phi$ energy ratio

$$
\begin{equation*}
R_{\phi}=\frac{E_{3 \times 3}^{S 2}}{E_{3 \times 7}^{S 2}} \tag{A3}
\end{equation*}
$$

is defined similarly to $R_{\eta}$. $R_{\phi}$ behaves very differently for unconverted and converted photons, since the electrons and positrons generated by the latter bend in different directions in $\phi$ because of the solenoid magnetic field, producing larger showers in the $\phi$ direction than the unconverted photons.
(c) Middle lateral width

$$
\begin{equation*}
w_{2}=\sqrt{\frac{\sum E_{i} \eta_{i}^{2}}{\sum E_{i}}-\left(\frac{\sum E_{i} \eta_{i}}{\sum E_{i}}\right)^{2}} \tag{A4}
\end{equation*}
$$

measures the shower lateral width in the second layer of the electromagnetic calorimeter, using all cells in a window $\eta \times \phi=3 \times 5$ measured in cell units.
(3) Variables using the first ("front") layer of the electromagnetic calorimeter
The discriminating variables based on the energy deposited in the first layer of the electromagnetic calorimeter are the following:
(a) Front side energy ratio

$$
\begin{equation*}
F_{\text {side }}=\frac{E( \pm 3)-E( \pm 1)}{E( \pm 1)} \tag{A5}
\end{equation*}
$$

measures the lateral containment of the shower, along the $\eta$ direction. $E( \pm n)$ is the energy in the $\pm n$ strip cells around the one with the largest energy.
(b) Front lateral width (3 strips)

$$
\begin{equation*}
w_{s, 3}=\sqrt{\frac{\sum E_{i}\left(i-i_{\max }\right)^{2}}{\sum E_{i}}} \tag{A6}
\end{equation*}
$$

measures the shower width along $\eta$ in the first layer of the electromagnetic calorimeter, using two strip cells around the maximal energy deposit. The index $i$ is the strip identification number, $i_{\text {max }}$ identifies the strip cells with the greatest energy, $E_{i}$ is the energy deposit in each strip cell.
(c) Front lateral width (total)
$w_{s, \text { tot }}$ measures the shower width along $\eta$ in the first layer of the electromagnetic calorimeter using all

TABLE III. The measured isolated prompt photon production cross section, for $0.00 \leq\left|\eta^{\gamma}\right|<0.60$. The systematic uncertainties originating from the purity measurement, the photon selection, the photon energy scale, the unfolding procedure and the luminosity are shown. The total uncertainty includes both the statistical and all systematic uncertainties, except for the uncertainty on the luminosity.

| $E_{\text {T }}^{\gamma}$ | $\frac{d \sigma}{d E_{\mathrm{T}}^{\top}}$ | stat | Measured |  |  |  |  |  | JETPHOX |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | $\begin{aligned} & \text { syst } \\ & \text { (purity) } \end{aligned}$ | $\begin{gathered} \text { syst } \\ \text { (efficiency) } \end{gathered}$ | $\begin{gathered} \text { syst } \\ \text { (en. scale) } \end{gathered}$ | $\begin{gathered} \text { syst } \\ \text { (unfolding) } \end{gathered}$ | $\begin{gathered} \text { syst } \\ \text { (luminosity) } \end{gathered}$ | total uncertainty | $\frac{d \sigma}{d E_{\mathrm{T}}^{\top}}$ | total uncertainty |
| [GeV] | [nb/GeV] | [nb/GeV] | [nb/GeV] | [nb/GeV] | [ $\mathrm{nb} / \mathrm{GeV}$ ] | [ $\mathrm{nb} / \mathrm{GeV}$ ] | [ $\mathrm{nb} / \mathrm{GeV}$ ] | [ $\mathrm{nb} / \mathrm{GeV}$ ] | [nb/GeV] | [nb/GeV] |
| $[15,20)$ | 5.24 | $\pm 0.11$ | ${ }_{-0.88}^{+0.52}$ | $\pm 0.81$ | +0.51 ${ }_{-0.46}$ | $\pm 0.11$ | $\pm 0.58$ | ${ }_{-1.4}^{+1.3}$ | 6.8 | ${ }_{-0.9}^{+1.4}$ |
| $[20,25)$ | 1.88 | $\pm 0.05$ | ${ }^{+0.18}$ | $\pm 0.21$ | ${ }_{-0.14}^{+0.14}$ | $\pm 0.04$ | $\pm 0.21$ | $\pm 0.36$ | 2.38 | ${ }_{-0.30}^{+0.45}$ |
| $[25,30)$ | 0.88 | $\pm 0.03$ | $\pm 0.07$ | $\pm 0.08$ | $\begin{array}{r}+0.09 \\ { }_{-0.08} \\ \hline 0.014\end{array}$ | $\pm 0.02$ | $\pm 0.10$ | ${ }_{-0.15}^{+0.16}$ | 1.01 | +0.17 |
| $[30,35)$ | 0.461 | $\pm 0.016$ | ${ }_{-0.019}^{+0.029}$ | $\pm 0.035$ | ${ }_{-0.046}^{+0.045}$ | $\pm 0.009$ | $\pm 0.05$ | $\pm 0.07$ | 0.50 | ${ }_{-0.04}^{+0.10}$ |
| $[35,40)$ | 0.254 | $\pm 0.011$ | ${ }_{-0.015}^{+0.017}$ | $\pm 0.019$ | ${ }_{-0.025}^{+0.027}$ | $\pm 0.005$ | $\pm 0.028$ | $\pm 0.04$ | 0.28 | ${ }_{-0.03}^{+0.04}$ |
| [40, 50) | 0.115 | $\pm 0.005$ | ${ }_{-0.006}^{+0.008}$ | $\pm 0.007$ | ${ }_{-0.009}^{+0.009}$ | $\pm 0.0023$ | $\pm 0.013$ | ${ }_{-0.016}^{+0.017}$ | 0.127 | ${ }_{-0.014}^{+0.018}$ |
| $[50,60)$ | 0.050 | $\pm 0.003$ | ${ }_{-0.002}^{+0.003}$ | $\pm 0.003$ | ${ }^{+}+0.0005$ | $\pm 0.001$ | $\pm 0.005$ | ${ }_{-0.007}^{+0.008}$ | 0.052 | ${ }_{-0.006}^{+0.007}$ |
| [60, 100) | 0.0120 | $\pm 0.0007$ | $\begin{array}{r} +0.0007 \\ \hline-0.0005 \\ \hline \end{array}$ | $\pm 0.0006$ | $\begin{array}{r} +0.001 \\ \hline-0.0012 \\ \hline \end{array}$ | $\pm 0.0002$ | $\pm 0.0013$ | $\begin{array}{r} +0.0019 \\ \hline-0.0018 \end{array}$ | 0.0121 | ${ }_{-0.0012}^{+0.0014}$ |

TABLE IV. The measured isolated prompt photon production cross section, for $0.60 \leq\left|\eta^{\gamma}\right|<1.37$. The systematic uncertainties originating from the purity measurement, the photon selection, the photon energy scale, the unfolding procedure and the luminosity are shown. The total uncertainty includes both the statistical and all systematic uncertainties, except for the uncertainty on the luminosity.

| $E_{\mathrm{T}}^{\gamma}$ | $\frac{d \sigma}{d E_{\mathrm{T}}^{7}}$ | stat | Measured |  |  |  |  | total uncertainty [nb/GeV] | JETPHOX |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | $\begin{gathered} \text { syst } \\ \text { (purity) } \\ {[\mathrm{nb} / \mathrm{GeV}]} \end{gathered}$ |  | $\begin{gathered} \text { syst } \\ \text { (en. scale) } \\ {[\mathrm{nb} / \mathrm{GeV}]} \end{gathered}$ | $\begin{gathered} \text { syst } \\ \text { (unfolding) } \\ {[\mathrm{nb} / \mathrm{GeV}]} \end{gathered}$ | syst (luminosity) $[\mathrm{nb} / \mathrm{GeV}]$ |  | $\begin{gathered} \frac{d \sigma}{d E_{\mathrm{T}}^{\nu}} \\ {[\mathrm{nb} / \mathrm{GeV}]} \\ \hline \end{gathered}$ | total uncertainty [nb/GeV] |
| $[15,20)$ | 5.9 | $\pm 0.2$ | ${ }_{-0.8}^{+1.8}$ | $\pm 1.0$ | ${ }_{-0.5}^{+0.6}$ | $\pm 0.1$ | $\pm 0.6$ | ${ }_{-1.4}^{+2.3}$ | 8.5 | ${ }_{-1.7}^{+1.7}$ |
| $[20,25)$ | 2.23 | $\pm 0.07$ | +0.49 -0.18 | $\pm 0.28$ | ${ }_{-0.16}^{+0.16}$ | $\pm 0.04$ | $\pm 0.24$ | ${ }_{-0 .}^{+0.6}$ | 3.0 | ${ }_{-0.5}^{+0.5}$ |
| $[25,30)$ | 1.05 | $\pm 0.03$ | ${ }_{-0.06}^{+0.16}$ | $\pm 0.10$ | ${ }_{-0.10}^{+0.10}$ | $\pm 0.021$ | $\pm 0.12$ | -0.24 | 1.28 | ${ }_{-}^{+0.18}$ |
| $[30,35)$ | 0.52 | $\pm 0.02$ | ${ }_{-0.03}^{+0.06}$ | $\pm 0.04$ | ${ }_{-0.05}^{+0.05}$ | $\pm 0.011$ | $\pm 0.06$ | ${ }_{-0.09}^{+0.11}$ | 0.64 | +0.11 -0.09 |
| $[35,40)$ | 0.313 | $\pm 0.014$ | ${ }_{-0.021}^{+0.029}$ | $\pm 0.024$ | ${ }_{-0.032}^{+0.035}$ | $\pm 0.006$ | $\pm 0.034$ | ${ }_{-0.05}^{+0.06}$ | 0.344 | ${ }_{-0.039}^{+0.052}$ |
| $[40,50)$ | 0.146 | $\pm 0.006$ | ${ }_{-0.011}^{+0.0014}$ | $\pm 0.009$ | ${ }_{-0.013}^{+0.0013}$ | $\pm 0.003$ | $\pm 0.016$ | ${ }_{-0.022}^{+0.025}$ | 0.161 | ${ }_{-0.019}^{+0.022}$ |
| [50, 60] | 0.062 | $\pm 0.004$ | ${ }_{-0.004}^{+0.005}$ | $\pm 0.003$ | ${ }_{-0.006}^{+0.006}$ | $\pm 0.001$ | $\pm 0.007$ | ${ }^{+}{ }^{+0.0009}$ | 0.065 | ${ }_{-0.007}^{+0.009}$ |
| [60, 100) | 0.0138 | $\pm 0.0008$ | ${ }^{-}+0.0001300013$ | $\pm 0.0007$ | $\begin{array}{r} 0.0016 \\ +0.0016 \end{array}$ | $\pm 0.0003$ | $\pm 0.0015$ | $\begin{array}{r} -0.0025 \\ +0.0025 \end{array}$ | 0.0154 | - ${ }_{-0.0015}^{+0.0019}$ |

TABLE V. The measured isolated prompt photon production cross section, for $1.52 \leq\left|\eta^{\gamma}\right|<1.81$. The systematic uncertainties originating from the purity measurement, the photon selection, the photon energy scale, the unfolding procedure and the luminosity are shown. The total uncertainty includes both the statistical and all systematic uncertainties, except for the uncertainty on the luminosity.

| $E_{T}^{\gamma}$ | $\frac{d \sigma}{d E_{\mathrm{T}}^{0}}$ | stat | Measured |  |  | $\begin{gathered} \text { syst } \\ \text { (unfolding) } \end{gathered}$ | $\begin{gathered} \text { syst } \\ \text { (luminosity) } \end{gathered}$ | total uncertainty [nb/GeV] | JETPHOX |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | syst <br> (purity) <br> [nb/GeV] | syst (efficiency) | $\begin{gathered} \text { syst } \\ \text { (en. scale) } \\ {[\mathrm{nb} / \mathrm{GeV}]} \end{gathered}$ |  |  |  | $\frac{d \sigma}{d E_{\mathrm{T}}^{\top}}$ | total uncertainty [nb/GeV] |
| $[15,20)$ | 2.9 | $\pm 0.1$ | ${ }_{-0.8}^{+0.8}$ | $\pm 0.5$ | ${ }_{-0.3}$ | $\pm 0.1$ | $\pm 0.3$ | ${ }^{+1.1}$ | 3.1 | 0.6 |
| $[20,25)$ | 1.12 | $\pm 0.04$ | ${ }_{-0}^{+0.15}$ | $\pm 0.16$ | ${ }^{+0.08}$ | $\pm 0.02$ | $\pm 0.12$ | ${ }_{+}^{-0.7}{ }_{-0.27}^{+0.27}$ | 1.10 | -0.5 +0.20 -0.15 |
| $[25,30)$ | 0.47 | $\pm 0.02$ | ${ }_{-}^{+0.04}$ | $\pm 0.05$ | ${ }^{-0.08}{ }_{-0.04}^{+0.05}$ | $\pm 0.01$ | $\pm 0.05$ | -0.24 ${ }_{-0.09}^{+0.11}$ | 0.46 | ${ }_{-}^{-0.07}+{ }_{-0.06}^{+0.07}$ |
| $[30,35)$ | 0.240 | $\pm 0.013$ | ${ }_{-0.016}^{+0.028}$ | $\pm 0.023$ | ${ }_{-0.026}^{+0.025}$ | $\pm 0.005$ | $\pm 0.026$ | ${ }_{-0.045}^{+0.052}$ | 0.233 | ${ }_{-0.030}^{+0.037}$ |
| $[35,40)$ | 0.142 | $\pm 0.009$ | ${ }_{-0.010}^{+0.0018}$ | $\pm 0.012$ | ${ }^{-}{ }^{+0.0014}$ | $\pm 0.0032$ | $\pm 0.016$ | ${ }^{+}{ }_{-0.026}^{+0.030}$ | 0.126 | ${ }^{-0.020}$ |
| [40, 50) | 0.062 | $\pm 0.004$ | ${ }_{-0.004}^{+0.005}$ | $\pm 0.005$ | ${ }^{+}+0.0006$ | $\pm 0.0013$ | $\pm 0.007$ | ${ }_{-0.010}^{+0.0011}$ | 0.058 | ${ }_{-0.007}^{+0.008}$ |
| $[50,60)$ | 0.0237 | $\pm 0.0025$ | ${ }_{-0.0028}^{+0.0026}$ | $\pm 0.0019$ | ${ }_{-0.0022}^{+0.0024}$ | $\pm 0.0005$ | $\pm 0.003$ | $\pm 0.005$ | 0.0243 | - ${ }_{-0.0027}^{+0.0033}$ |
| [60, 100) | 0.0066 | $\pm 0.0005$ | $\begin{array}{r} +0.0000 \\ -0.0003 \\ -0.003 \end{array}$ | $\pm 0.0005$ | $\begin{array}{r} +0.0008 \\ -0.0007 \\ -0.00 \end{array}$ | $\pm 0.0002$ | $\pm 0.0007$ | $\begin{aligned} & +0.0013 \\ & -0.0012 \end{aligned}$ | 0.0057 | +0.0007 ${ }_{-0.0006}$ |

cells in a window $\Delta \eta \times \Delta \phi=0.0625 \times 0.2$, corresponding approximately to $20 \times 2$ strip cells in $\eta \times \phi$, and is computed as $w_{s, 3}$.
(d) Front second maximum difference.

$$
\begin{equation*}
\Delta E=\left[E_{2^{\text {nd }} \max }^{S 1}-E_{\min }^{S 1}\right] \tag{A7}
\end{equation*}
$$

is the difference between the energy of the strip cell with the second greatest energy $E_{2^{\text {nd }} \text { max }}^{S 1}$, and the energy in the strip cell with the least energy found between the greatest and the second greatest energy $E_{\min }^{S 1}(\Delta E=0$ when there is no second maximum).
(e) Front maxima relative ratio
measures the relative difference between the energy of the strip cell with the greatest energy $E_{1^{\text {st }} \max }^{S 1}$ and the energy in the strip cell with second greatest energy $E_{2^{\text {nd }} \max }^{\text {n }^{1}}$ ( 1 when there is no second maximum).

## APPENDIX B: CROSS SECTION MEASUREMENTS

Table III, IV, and V list the values of the measured isolated prompt photon production cross sections, for the $0.00 \leq\left|\eta^{\gamma}\right|<0.60,0.60 \leq\left|\eta^{\gamma}\right|<1.37$ and $1.52 \leq$ $\left|\eta^{\gamma}\right|<1.81$ regions, respectively. The various systematic uncertainties originating from the purity measurement, the photon selection and identification efficiency, the photon energy scale and the luminosity are shown. The total uncertainty includes both the statistical and all systematic uncertainties, except for the uncertainty on the luminosity.
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V. B. Bobrovnikov, ${ }^{107}$ A. Bocci, ${ }^{44}$ R. Bock, ${ }^{29}$ C. R. Boddy, ${ }^{118}$ M. Boehler, ${ }^{41}$ J. Boek, ${ }^{174}$ N. Boelaert, ${ }^{35}$ S. Böser, ${ }^{77}$ J. A. Bogaerts,,$^{29}$ A. Bogdanchikov, ${ }^{107}$ A. Bogouch, ${ }^{90, a}$ C. Bohm, ${ }^{146 a}$ V. Boisvert, ${ }^{76}$ T. Bold, ${ }^{163, f}$ V. Boldea, ${ }^{25 a}$ M. Bona, ${ }^{75}$ M. Boonekamp, ${ }^{136}$ G. Boorman, ${ }^{76}$ C. N. Booth, ${ }^{139}$ P. Booth, ${ }^{139}$ J. R. A. Booth, ${ }^{17}$ S. Bordoni, ${ }^{78}$ C. Borer, ${ }^{16}$
A. Borisov, ${ }^{128}$ G. Borissov, ${ }^{71}$ I. Borjanovic, ${ }^{12 \mathrm{a}}$ S. Borroni, ${ }^{132 \mathrm{a}, 132 \mathrm{~b}} \mathrm{~K}$. Bos, ${ }^{105}$ D. Boscherini, ${ }^{19 \mathrm{a}}$ M. Bosman, ${ }^{11}$ H. Boterenbrood, ${ }^{105}$ D. Botterill, ${ }^{129}$ J. Bouchami, ${ }^{93}$ J. Boudreau, ${ }^{123}$ E. V. Bouhova-Thacker, ${ }^{71}$ C. Boulahouache, ${ }^{123}$ C. Bourdarios, ${ }^{115}$ N. Bousson,,$^{83}$ A. Boveia, ${ }^{30}$ J. Boyd, ${ }^{29}$ I. R. Boyko, ${ }^{65}$ N. I. Bozhko, ${ }^{128}$ I. Bozovic-Jelisavcic, ${ }^{12 b}$ S. Braccini, ${ }^{47}$ J. Bracinik, ${ }^{17}$ A. Braem, ${ }^{29}$ E. Brambilla, ${ }^{72 \mathrm{a}, 72 \mathrm{~b}}$ P. Branchini, ${ }^{134 \mathrm{a}}$ G. W. Brandenburg, ${ }^{57}$ A. Brandt, ${ }^{7}$ G. Brandt, ${ }^{41}$ O. Brandt, ${ }^{54}$ U. Bratzler, ${ }^{156}$ B. Brau, ${ }^{84}$ J. E. Brau, ${ }^{114}$ H. M. Braun, ${ }^{174}$ B. Brelier, ${ }^{158}$ J. Bremer, ${ }^{29}$ R. Brenner, ${ }^{166}$ S. Bressler, ${ }^{152}$ D. Breton, ${ }^{115}$ N. D. Brett, ${ }^{118}$ P. G. Bright-Thomas, ${ }^{17}$ D. Britton, ${ }^{53}$ F. M. Brochu, ${ }^{27}$
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# Measurement of the isolated diphoton cross section in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

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#### Abstract

The ATLAS experiment has measured the production cross section of events with two isolated photons in the final state, in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$. The full data set acquired in 2010 is used, corresponding to an integrated luminosity of $37 \mathrm{pb}^{-1}$. The background, consisting of hadronic jets and isolated electrons, is estimated with fully data-driven techniques and subtracted. The differential cross sections, as functions of the di-photon mass ( $m_{\gamma \gamma}$ ), total transverse momentum ( $p_{\mathrm{T}, \gamma \gamma}$ ), and azimuthal separation $\left(\Delta \phi_{\gamma \gamma}\right)$, are presented and compared to the predictions of next-to-leading-order QCD.


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## I. INTRODUCTION

The production of di-photon final states in protonproton collisions may occur through quark-antiquark $t$-channel annihilation, $q \bar{q} \rightarrow \gamma \gamma$, or via gluon-gluon interactions, $g g \rightarrow \gamma \gamma$, mediated by a quark box diagram. Despite the higher order of the latter, the two contributions are comparable, due to the large gluon flux at the LHC. Photon-parton production with photon radiation also contributes in processes such as $q \bar{q}, g g \rightarrow g \gamma \gamma$, and $q g \rightarrow q \gamma \gamma$. During the parton fragmentation process, more photons may also be produced. In this analysis, all such photons are considered as signal if they are isolated from other activity in the event. Photons produced after the hadronization by neutral hadron decays, or coming from radiative decays of other particles, are considered as part of the background.

The measurement of the di-photon production crosssection at the LHC is of great interest as a probe of QCD, especially in some particular kinematic regions. For instance, the distribution of the azimuthal separation, $\Delta \phi_{\gamma \gamma}$, is sensitive to the fragmentation model, especially when both photons originate from fragmentation. On the other hand, for balanced back-to-back di-photons ( $\Delta \phi_{\gamma \gamma} \simeq$ $\pi$ and small total transverse momentum, $p_{\mathrm{T}, \gamma \gamma}$ ) the production is sensitive to soft gluon emission, which is not accurately described by fixed-order perturbation theory.

Di-photon production is also an irreducible background for some new physics processes, such as the Higgs decay into photon pairs [1]: in this case, the spectrum of the invariant mass, $m_{\gamma \gamma}$, of the pair is analyzed, searching for a resonance. Moreover, di-photon production is a
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characteristic signature of some exotic models beyond the standard model. For instance, universal extra dimensions predict nonresonant di-photon production associated with significant missing transverse energy [2,3]. Other extra-dimension models, such as Randall-Sundrum [4], predict the production of gravitons, which would decay into photon pairs with a narrow width.

Recent cross-section measurements of di-photon production at hadron colliders have been performed by the D0 [5] and CDF [6] collaborations, at the Tevatron protonantiproton collider with a center-of-mass energy $\sqrt{s}=$ 1.96 TeV .

In this document, di-photon production is studied in proton-proton collisions at the LHC, with a center-ofmass energy $\sqrt{s}=7 \mathrm{TeV}$. After a short description of the ATLAS detector (Sec. II), the analyzed collision data and the event selection are detailed in Sec. III, while the supporting simulation samples are listed in Sec. IV. The isolation properties of the signal and of the hadronic background are studied in Sec. V. The evaluation of the di-photon signal yield is obtained by subtracting the backgrounds from hadronic jets and from isolated electrons, estimated with data-driven methods as explained in Sec. VI. Section VII describes how the event selection efficiency is evaluated and how the final yield is obtained. Finally, in Sec. VIII, the differential cross-section of diphoton production is presented as a function of $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}$, and $\Delta \phi_{\gamma \gamma}$.

## II. THE ATLAS DETECTOR

The ATLAS detector [7] is a multipurpose particle physics apparatus with a forward-backward symmetric cylindrical geometry and near $4 \pi$ coverage in solid angle. ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the center of the detector and the $z$ axis along the beam pipe. The $x$ axis points from the IP to the center of the LHC ring, and the $y$ axis points upward. Cylindrical coordinates $(r, \phi)$ are
used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta=-\ln [\tan (\theta / 2)]$. The transverse momentum is defined as $p_{T}=p \sin \theta=$ $p / \cosh \eta$, and a similar definition holds for the transverse energy $E_{\mathrm{T}}$.

The inner tracking detector (ID) covers the pseudorapidity range $|\eta|<2.5$ and consists of a silicon pixel detector, a silicon microstrip detector, and a transition radiation tracker in the range $|\eta|<2.0$. The ID is surrounded by a superconducting solenoid providing a 2 T magnetic field. The inner detector allows an accurate reconstruction of tracks from the primary proton-proton collision region and also identifies tracks from secondary vertices, permitting the efficient reconstruction of photon conversions in the inner detector up to a radius of $\approx 80 \mathrm{~cm}$.

The electromagnetic calorimeter (ECAL) is a leadliquid argon (LAr) sampling calorimeter with an accordion geometry. It is divided into a barrel section, covering the pseudorapidity region $|\eta|<1.475$, and two endcap sections, covering the pseudorapidity regions $1.375<|\eta|<$ 3.2. It consists of three longitudinal layers. The first one, in the ranges $|\eta|<1.4$ and $1.5<|\eta|<2.4$, is segmented into high granularity "strips" in the $\eta$ direction, sufficient to provide an event-by-event discrimination between single photon showers and two overlapping showers coming from a $\pi^{0}$ decay. The second layer of the electromagnetic calorimeter, which collects most of the energy deposited in the calorimeter by the photon shower, has a thickness of about 17 radiation lengths and a granularity of $0.025 \times 0.025$ in $\eta \times \phi$ (corresponding to one cell). A third layer is used to correct leakage beyond the ECAL for high-energy showers. In front of the accordion calorimeter a thin presampler layer, covering the pseudorapidity interval $|\eta|<1.8$, is used to correct for energy loss before the calorimeter.

The hadronic calorimeter (HCAL), surrounding the ECAL, consists of an iron-scintillator tile calorimeter in the range $|\eta|<1.7$ and two copper-LAr calorimeters spanning $1.5<|\eta|<3.2$. The acceptance is extended by two tungsten-LAr forward calorimeters up to $|\eta|<4.9$. The muon spectrometer, located beyond the calorimeters, consists of three large air-core superconducting toroid systems, precision tracking chambers providing accurate muon tracking over $|\eta|<2.7$, and fast detectors for triggering over $|\eta|<2.4$.

A three-level trigger system is used to select events containing two photon candidates. The first level trigger (level-1) is hardware based: using a coarser cell granularity ( $0.1 \times 0.1$ in $\eta \times \phi$ ), it searches for electromagnetic deposits with a transverse energy above a programmable threshold. The second and third level triggers (collectively referred to as the "high-level" trigger) are implemented in software and exploit the full granularity and energy calibration of the calorimeter.

## III. COLLISION DATA AND SELECTIONS

The analyzed data set consists of proton-proton collision data at $\sqrt{s}=7 \mathrm{TeV}$ collected in 2010, corresponding to an integrated luminosity of $37.2 \pm 1.3 \mathrm{pb}^{-1}$ [8]. The events are considered only when the beam condition is stable and the trigger system, the tracking devices, and the calorimeters are operational.

## A. Photon reconstruction

A photon is defined starting from a cluster in the ECAL. If there are no tracks pointing to the cluster, the object is classified as an unconverted photon. In case of converted photons, one or two tracks may be associated to the cluster, thereby creating an ambiguity in the classification with respect to electrons. This is addressed as described in Ref [9].

A fiducial acceptance is required in pseudorapidity, $\left|\eta^{\gamma}\right|<2.37$, with the exclusion of the barrel/endcap transition $1.37<\left|\eta^{\gamma}\right|<1.52$. This corresponds to the regions where the ECAL strips granularity is more effective for photon identification and jet background rejection [9]. Moreover, photons reconstructed near to regions affected by readout or high-voltage failures are not considered.

In the considered acceptance range, the uncertainty on the photon energy scale is estimated to be $\sim \pm 1 \%$. The energy resolution is parametrized as $\sigma_{E} / E \simeq a / \sqrt{E[\mathrm{GeV}]}$ $\oplus c$, where the sampling term $a$ varies between $10 \%$ and $20 \%$ depending on $\eta^{\gamma}$, and the constant term $c$ is estimated to be $1.1 \%$ in the barrel and $1.8 \%$ in the endcap. Such a performance has been measured in $Z \rightarrow e^{+} e^{-}$events observed in proton-proton collision data in 2010.

## B. Photon selection

The photon sample suffers from a major background due to hadronic jets, which generally produce calorimetric deposits broader and less isolated than electromagnetic showers, with sizable energy leaking to the HCAL. Most of the background is reduced by applying requirements (referred to as the LOOSE selection, $\mathbf{L}$ ) on the energy fraction measured in the HCAL, and on the shower width measured by the second layer of the ECAL. The remaining background is mostly due to photon pairs from neutral hadron decays (mainly $\pi^{0}$ ) with a small opening angle and reconstructed as single photons. This background is further reduced by applying a more stringent selection on the shower width in the second ECAL layer, together with additional requirements on the shower shape measured by the first ECAL layer: a narrow shower width and the absence of a second significant maximum in the energy deposited in contiguous strips. The combination of all these requirements is referred to as the TIGHT selection (T). Since converted photons tend to have broader shower shapes than unconverted ones, the cuts of the TIGHT selection are tuned differently for the two photon categories.

More details on these selection criteria are given in Ref. [10].

To reduce the jet background further, an isolation requirement is applied: the isolation transverse energy $E_{\mathrm{T}}^{\text {iso }}$, measured by the calorimeters in a cone of angular radius $R=\sqrt{\left(\eta-\eta^{\gamma}\right)^{2}+\left(\phi-\phi^{\gamma}\right)^{2}}<0.4$, is required to satisfy $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$ (isolated photon, $\mathbf{I}$ ). The calculation of $E_{\mathrm{T}}^{\text {iso }}$ is performed summing over ECAL and HCAL cells surrounding the photon candidate, after removing a central core that contains most of the photon energy. An out-ofcore energy correction [10] is applied, to make $E_{\mathrm{T}}^{\text {iso }}$ essentially independent of $E_{\mathrm{T}}^{\gamma}$, and an ambient energy correction, based on the measurement of soft jets [11,12] is applied on an event-by-event basis, to remove the contribution from the underlying event and from additional proton-proton interactions ("in-time pile-up").

## C. Event selection

The di-photon candidate events are selected according to the following steps:
(i) The events are selected by a di-photon trigger, in which both photon candidates must satisfy the trigger selection and have a transverse energy $E_{\mathrm{T}}^{\gamma}>$ 15 GeV . To select genuine collisions, at least one primary vertex with three or more tracks must be reconstructed.
(ii) The event must contain at least two photon candidates, with $E_{\mathrm{T}}^{\gamma}>16 \mathrm{GeV}$, in the acceptance defined in Sec. III A and passing the LOOSE selection. If more than two such photons exist, the two with highest $E_{\mathrm{T}}^{\gamma}$ are chosen.
(iii) To avoid a too large overlap between the two isolation cones, an angular separation $\Delta R_{\gamma \gamma}=$ $\sqrt{\left(\eta_{1}^{\gamma}-\eta_{2}^{\gamma}\right)^{2}+\left(\phi_{1}^{\gamma}-\phi_{2}^{\gamma}\right)^{2}}>0.4$ is required.
(iv) Both photons must satisfy the TIGHT selection (TT sample).
(v) Both photons must satisfy the isolation requirement $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$ (TITI sample).

In the analyzed data set, there are 63673 events where both photons satisfy the LOOSE selection and the $\Delta R_{\gamma \gamma}$ separation requirement. Among these, 5365 events belong to the TT sample, and 2022 to the TITI sample.

## IV. SIMULATED EVENTS

The characteristics of the signal and background events are investigated with Monte Carlo samples, generated using PYTHIA 6.4.21 [13]. The simulated samples are generated with pile-up conditions similar to those under which most of the data were taken. Particle interactions with the detector materials are modeled with GEANT4 [14] and the detector response is simulated. The events are reconstructed with the same algorithms used for collision data.

More details on the event generation and simulation infrastructure are provided in Ref [15].

The di-photon signal is generated with PYTHIA, where photons from both hard scattering and quark bremsstrahlung are modeled. To study systematic effects due to the generator model, an alternative di-photon sample has been produced with SHERPA [16].

The background processes are generated with the main physical processes that produce (at least) two sizable calorimetric deposits: these include di-jet and photon-jet final states, but minor contributions, e.g. from $W, Z$ bosons, are also present. Such a Monte Carlo sample, referred to as "di-jet-like," provides a realistic mixture of the main final states expected to contribute to the selected data sample. Moreover, dedicated samples of $W \rightarrow e \nu$ and $Z \rightarrow e^{+} e^{-}$ simulated events are used for the electron/photon comparison in isolation and background studies.

## V. PROPERTIES OF THE ISOLATION TRANSVERSE ENERGY

The isolation transverse energy, $E_{\mathrm{T}}^{\text {iso }}$, is a powerful discriminating variable to estimate the jet background contamination in the sample of photon candidates. The advantage of using this quantity is that its distribution can be extracted directly from the observed collision data, both for the signal and the background, without relying on simulations.

Section VA describes a method to extract the distribution of $E_{\mathrm{T}}^{\text {iso }}$ for background and signal, from observed photon candidates. An independent method to extract the signal $E_{\mathrm{T}}^{\text {iso }}$ distribution, based on observed electrons, is described in Sec. V B. Finally, the correlation between isolation energies in events with two photon candidates is discussed in Sec. V C.

## A. Background and signal isolation from photon candidates

For the background study, a control sample is defined by reconstructed photons that fail the TIGHT selection but pass a looser one, where some cuts are released on the shower shapes measured by the ECAL strips. Such photons are referred to as NONTIGHT. A study carried out on the "di-jet-like" Monte Carlo sample shows that the $E_{\mathrm{T}}^{\text {iso }}$ distribution in the NONTIGHT sample reproduces that of the background, as shown in Fig. 1(a).

The TIGHT photon sample contains a mixture of signal and background. However, a comparison between the shapes of the $E_{\mathrm{T}}^{\text {iso }}$ distributions from TIGHT and NONTIGHT samples [Fig. 1(b)] shows that for $E_{\mathrm{T}}^{\text {iso }}>7 \mathrm{GeV}$ there is essentially no signal in the TIGHT sample. Therefore, the background contamination in the TIGHT sample can be subtracted by using the NONTIGHT sample, normalized such that the integrals of the two distributions are equal for $E_{\mathrm{T}}^{\text {iso }}>7 \mathrm{GeV}$. The $E_{\mathrm{T}}^{\text {iso }}$ distribution of the signal alone


FIG. 1 (color online). Extraction of the isolation energy ( $E_{\mathrm{T}}^{\text {iso }}$ ) distributions for signal and background. The plots are made with a "di-jet-like" Monte Carlo sample: the "signal" and "background" classifications are based on the Monte Carlo information. (a) Normalized $E_{\mathrm{T}}^{\text {iso }}$ distribution for the background and for the NONTIGHT sample. (b) $E_{\mathrm{T}}^{\text {iso }}$ distribution, for the TIGHT and the nontight samples: the latter is scaled as explained in the text. (c) Normalized $E_{\mathrm{T}}^{\text {iso }}$ distribution for the signal and for the TIGHT sample, after subtracting the scaled NONTIGHT sample. In ( $\mathrm{a}, \mathrm{c}$ ) the vertical line shows the isolation cut $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$.
is thus extracted. Figure 1(c) shows the result, for photons in the "di-jet-like" Monte Carlo sample.

In collision data, events with two photon candidates are used to build the TIGHT and NONTIGHT samples, for the leading and subleading candidate separately. The points in Fig. 2 display the distribution of $E_{\mathrm{T}}^{\text {iso }}$ for the leading and subleading photons. In each of the two distributions, one bin has higher content, reflecting opposing fluctuations in the subtracted input distributions in those bins. The effect on the di-photon cross-section measurement is negligible.

The main source of systematic error comes from the definition of the NONTIGHT control sample. There are three sets of strips cuts that could be released: the first set concerns the shower width in the core, the second tests for the presence of two maxima in the cluster, and the third is a cut on the full shower width in the strips. The choice adopted is to release only the first two sets of cuts, as the best compromise between maximizing the statistics in the control sample, while keeping the background $E_{\mathrm{T}}^{\text {iso }}$ distribution fairly unbiased. To test the effect of this choice, the sets of released cuts have been changed, either by releasing only the cuts on the shower core width in the strips, or by releasing all the strips cuts. A minor effect is also due to the choice of the region $E_{\mathrm{T}}^{\text {iso }}>7 \mathrm{GeV}$, to normalize the


FIG. 2 (color online). Data-driven signal isolation distributions for the leading (top) and subleading (bottom) photons obtained using the photon candidates (solid circles) or extrapolated from electrons (continuous lines).

NONTIGHT control sample: the cut has therefore been moved to 6 and 8 GeV .

More studies with the "di-jet-like" Monte Carlo sample have been performed, to test the robustness of the $E_{\mathrm{T}}^{\text {iso }}$ extraction against model-dependent effects such as (i) signal leakage into the NONTIGHT sample; (ii) correlations between $E_{\mathrm{T}}^{\text {iso }}$ and strips cuts; (iii) different signal composition, i.e. fraction of photons produced by the hard scattering or by the fragmentation process; (iv) different background composition, i.e. fraction of photon pairs from $\pi^{0}$ decays. In all cases, the overall systematic error, computed as described above, covers the differences between the true and data-driven results as evaluated from these Monte Carlo tests.

## B. Signal isolation from electron extrapolation

An independent method of extracting the $E_{\mathrm{T}}^{\text {iso }}$ distribution for the signal photons is provided by the "electron extrapolation." In contrast to photons, it is easy to select a pure electron sample from data, from $W^{ \pm} \rightarrow e^{ \pm} \nu$ and $Z \rightarrow$ $e^{+} e^{-}$events [17]. The main differences between the
electron and photon $E_{\mathrm{T}}^{\text {iso }}$ distributions are (i) the electron $E_{\mathrm{T}}^{\mathrm{iso}}$ in the bulk of the distribution is slightly larger, because of bremsstrahlung in the material upstream of the calorimeter; (ii) the photon $E_{\mathrm{T}}^{\text {iso }}$ distribution exhibits a larger tail because of the contribution of the photons from fragmentation, especially for the subleading photon. Such differences are quantified with $W^{ \pm} \rightarrow e^{ \pm} \nu, Z \rightarrow e^{+} e^{-}$, and $\gamma \gamma$ Monte Carlo samples by fitting the $E_{\mathrm{T}}^{\text {iso }}$ distributions with crystal ball functions [18] and comparing the parameters. Then, the electron/photon differences are propagated to the selected electrons from collision data. The result is shown by the continuous lines in Fig. 2, agreeing well with the $E_{\mathrm{T}}^{\text {iso }}$ distributions obtained from the NONTIGHT sample subtraction (circles).

## C. Signal and background isolation in events with two photon candidates

In events with two photon candidates, possible correlations between the two isolation energies have been investigated by studying the signal and background $E_{\mathrm{T}}^{\text {iso }}$ distributions of a candidate ("probe") under different isolation conditions of the other candidate ("tag"). The signal $E_{\mathrm{T}}^{\text {iso }}$ shows negligible dependence on the tag conditions. In contrast, the background $E_{\mathrm{T}}^{\mathrm{iso}}$ exhibits a clear positive correlation with the isolation transverse energy of the tag: if the tag passes (or fails) the isolation requirement, the probe background candidate is more (or less) isolated. This effect is visible especially in di-jet final states, which can be directly studied in collision data by requiring both photon candidates to be NONTIGHT, and is taken into account in the jet background estimation (Sec. VI A).

This correlation is also visible in the "di-jet-like" Monte Carlo sample.

## VI. BACKGROUND SUBTRACTION AND SIGNAL YIELD DETERMINATION

The main background to selected photon candidates consists of hadronic jets. This is reduced by the photon TIGHT selection described in Sec. III B. However a significant component is still present and must be subtracted. The techniques to achieve this are described in Sec. VI A.

Another sizable background component comes from isolated electrons, mainly originating from $W$ and $Z$ decays, which look similar to photons from the calorimetric point of view. The subtraction of such a contamination is addressed in Sec. VIB.

The background due to cosmic rays and to beam-gas collisions has been studied on dedicated data sets, selected by special triggers. Its impact is found to be negligible.

## A. Jet background

The jet background is due to photon-jet and di-jet final states. This section describes three methods, all based on
the isolation transverse energy, $E_{\mathrm{T}}^{\text {iso }}$, aiming to separate the TITI sample into four categories:


FIG. 3 (color online). Differential $\gamma \gamma$ yields in the TITI sample ( $N_{\gamma \gamma}^{\text {TITI }}$ ), as a function of the three observables $m_{\gamma \gamma}$, $p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$, obtained with the three methods. In each bin, the yield is divided by the bin width. The vertical error bars display the total errors, accounting for both the statistical uncertainties and the systematic effects. The points are artificially shifted horizontally, to better display the three results.
according to their physical final states- $\gamma \mathrm{j}$ and $\mathrm{j} \gamma$ differ by the jet faking, respectively, the subleading or the leading photon candidate. The signal yield $N_{\gamma \gamma}^{\text {TITI }}$ is evaluated in bins of the three observables $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$, as in Fig. 3. Because of the dominant back-to-back topology of di-photon events, the kinematic selection produces a turnon in the distribution of the di-photon invariant mass, at $m_{\gamma \gamma} \gtrsim 2 E_{\mathrm{T}}^{\text {cut }}$ ( $E_{\mathrm{T}}^{\text {cut }}=16 \mathrm{GeV}$ being the applied cut on the photon transverse energy), followed by the usual decrease typical of the continuum processes. The region at lower $m_{\gamma \gamma}$ is populated by di-photon events with low $\Delta \phi$.

The excess in the mass bin $80<m_{\gamma \gamma}<100 \mathrm{GeV}$, due to a contamination of electrons from Z-decays, is addressed in Sec. VI B.

From the evaluation of the background yields $\left(N_{\gamma \mathrm{j}}^{\text {TITI }}+\right.$ $N_{\mathrm{j} \gamma}^{\mathrm{TITI}}$ and $\left.N_{\mathrm{jj}}^{\mathrm{TITI}}\right)$, the average fractions of photon-jet and di-jet events in the TITI sample are $\sim 26 \%$ and $\sim 9 \%$, respectively.

The three results shown in Fig. 3 are compatible. This suggests that there are no hidden biases induced by the analyses. However, the three measures cannot be combined, as all make use of the same quantities- $E_{\mathrm{T}}^{\text {iso }}$ and shower shapes-and use the NONTIGHT background control region, so they may have correlations. None of the methods has striking advantages with respect to the others, and the systematic uncertainties are comparable. The "event weighting" method (Sec. VI A 1) is used for the crosssection evaluation, since it provides event weights that are also useful in the event efficiency evaluation, and its sources of systematic uncertainties are independent of those related to the signal modelling and reconstruction.

$$
\left(\begin{array}{cc}
\epsilon_{1} \epsilon_{2} & \epsilon_{1} f_{2} \\
\epsilon_{1}\left(1-\epsilon_{2}\right) & \epsilon_{1}\left(1-f_{2}\right) \\
\left(1-\epsilon_{1}\right) \epsilon_{2} & \left(1-\epsilon_{1}\right) f_{2} \\
\left(1-\epsilon_{1}\right)\left(1-\epsilon_{2}\right) & \left(1-\epsilon_{1}\right)\left(1-f_{2}\right)
\end{array}\right.
$$

where $\epsilon_{i}$ and $f_{i}(i=1,2$ for the leading/subleading candidate) are the probabilities that a signal or a fake photon, respectively, pass the isolation cut. These are obtained from the $E_{\mathrm{T}}^{\text {iso }}$ distributions extracted from collision data, as described in Sec. VA. The value of $\epsilon$ is essentially independent of $E_{\gamma}$ and changes with $\eta^{\gamma}$, ranging between $80 \%$ and $95 \%$. The value of $f$ depends on both $E_{\mathrm{T}}$ and $\eta$ and takes values between $20 \%$ and $40 \%$. Given such dependence on the kinematics, the matrix $\mathbf{E}^{(k)}$ is also evaluated for each event.

Because of the presence of correlation, the matrix coefficients in Eq. (2) actually involve conditional probabilities, depending on the pass/fail status of the other candidate (tag) of the pair. For instance, the first two coefficients in the last column become

## 1. Event weighting

Each event satisfying the TIGHT selection on both photons (sample TT) is classified according to whether the photons pass or fail the isolation requirement, resulting in a PP, PF, FP, or FF classification. These are translated into four event weights $W_{\gamma \gamma}, W_{\gamma \mathrm{j}}, W_{\mathrm{j} \gamma}, W_{\mathrm{jj}}$, which describe how likely the event is to belong to each of the four final states. A similar approach has already been used by the D0 [5] and CDF [6] collaborations.

The connection between the pass/fail outcome and the weights, for the $k$-th event, is:

$$
\left(\begin{array}{c}
S_{\mathrm{PP}}^{(k)}  \tag{1}\\
S_{\mathrm{PF}}^{(k)} \\
S_{\mathrm{FP}}^{(k)} \\
S_{\mathrm{FF}}^{(k)}
\end{array}\right)=\mathbf{E}^{(k)}\left(\begin{array}{c}
W_{\gamma \gamma}^{(k)} \\
W_{\gamma j}^{(k)} \\
W_{\mathrm{j} \gamma}^{(k)} \\
W_{\mathrm{jj}}^{(k)}
\end{array}\right) .
$$

If applied to a large number of events, the quantities $S_{X Y}$ would be the fractions of events satisfying each pass/fail classification, and the weights would be the fractions of events belonging to the four different final states. On an event-by-event approach, $S_{X Y}^{(k)}$ are boolean status variables (e.g. for an event where both candidates are isolated, $S_{\mathrm{PP}}^{(k)}=$ 1 and $S_{\mathrm{PF}}^{(k)}=S_{\mathrm{FP}}^{(k)}=S_{\mathrm{FF}}^{(k)}=0$ ). The quantity $\mathbf{E}^{(k)}$ is a $4 \times 4$ matrix, whose coefficients give the probability that a given final state produces a certain pass/fail status. If there were no correlation between the isolation transverse energies of the two candidates, it would have the form
$\left.\begin{array}{cc}f_{1} \epsilon_{2} & f_{1} f_{2} \\ f_{1}\left(1-\epsilon_{2}\right) & f_{1}\left(1-f_{2}\right) \\ \left(1-f_{1}\right) \epsilon_{2} & \left(1-f_{1}\right) f_{2} \\ \left(1-f_{1}\right)\left(1-\epsilon_{2}\right) & \left(1-f_{1}\right)\left(1-f_{2}\right)\end{array}\right)$,

$$
\begin{aligned}
f_{1} f_{2} & \rightarrow \frac{1}{2}\left[f_{1}^{\hat{\mathrm{P}}} f_{2}+f_{1} f_{2}^{\hat{\mathrm{P}}}\right] \\
f_{1}\left(1-f_{2}\right) & \rightarrow \frac{1}{2}\left[f_{1}^{\hat{\mathrm{P}}}\left(1-f_{2}\right)+f_{1}\left(1-f_{2}^{\hat{\mathrm{P}}}\right)\right]
\end{aligned}
$$

where the superscripts $\hat{P}$ and $\hat{F}$ denote the pass/fail status of the tag. The ambiguity in the choice of the tag is solved by taking both choices and averaging them. All the conditional $\left(\epsilon_{i}^{\hat{P}, \hat{F}}, f_{i}^{\hat{\mathrm{P}}, \hat{\mathrm{F}}}\right)$ probabilities are derived from collision data, as discussed in Sec. V C.

The signal yield in the TITI sample can be computed as a sum of weights running over all events in the TT sample:

$$
\begin{equation*}
N_{\gamma \gamma}^{\mathbf{T I T I}}=\sum_{k \in \mathbf{T} \mathbf{T}} w^{(k)} \pm \sqrt{\sum_{k \in \mathbf{T} \mathbf{T}}\left[w^{(k)}\right]^{2}} \tag{3}
\end{equation*}
$$

where the weight $w^{(k)}$ for the $k$ th event is

$$
\begin{equation*}
w^{(k)}=W_{\gamma \gamma}^{(k)} \epsilon_{1}^{(k)} \epsilon_{2}^{(k)} \tag{4}
\end{equation*}
$$

and the sum over $k$ is carried out on the events in a given bin of the variable of interest ( $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$ ). The result is shown in Fig. 3, by the solid circles.

The main sources of systematic errors are (i) the definition of the NONTIGHT control sample: ${ }_{-9 \%}^{+12 \%}$; (ii) the normalization of the NONTIGHT sample: ${ }_{-2 \%}^{+0}$; (iii) the statistics used to compute the $E_{\mathrm{T}}^{\text {iso }}$ distributions, and hence the precision of the matrix coefficients: $\pm 9 \%$. Effects (i) and (ii) are estimated as explained in Sec. VA. Effect (iii) is quantified by increasing and decreasing the $\epsilon, f$ parameters by their statistical errors and recomputing the signal yield: the variations are then added in quadrature.

## 2. Two-dimensional fit

From all the di-photon events satisfying the TIGHT selection (sample TT), the observed 2-dimensional distribution $F^{\mathrm{obs}}\left(E_{\mathrm{T}, 1}^{\text {iso }}, E_{\mathrm{T}, 2}^{\text {iso }}\right)$ of the isolation energies of the leading and subleading photons is built. Then, a linear combination of four unbinned probability density functions (PDFs), $F_{\gamma \gamma}, F_{\gamma \mathrm{j}}, F_{\mathrm{j} \gamma}, F_{\mathrm{jj}}$, describing the 2-dimensional distributions of the four final states, is fit to the observed distribution. For the $\gamma \gamma, \gamma \mathrm{j}, \mathrm{j} \gamma$ final states, the correlation between $E_{\mathrm{T}, 1}^{\mathrm{iso}}$ and $E_{\mathrm{T}, 2}^{\mathrm{iso}}$ is assumed to be negligible; therefore, the 2-dimensional PDFs are factorized into the leading and subleading PDFs. The leading and subleading photon PDFs $F_{\gamma_{1}}, F_{\gamma_{2}}$ are obtained from the electron extrapolation, as described in Sec. V B. The background PDF $F_{\mathrm{j}_{2}}$ for $\gamma \mathrm{j}$ events is obtained from the NONTIGHT sample on the subleading candidate, for events where the leading candidate satisfies the TIGHT selection. The background PDF $F_{\mathrm{j}_{1}}$ for $\mathrm{j} \gamma$ events is obtained in a similar way. Both background PDFs are then smoothed with empirical parametric functions. The PDF for jj events cannot be factorized, due to the sizable correlation between the two candidates. Therefore, a 2-dimensional PDF is directly extracted from events where both candidates belong to the NONTIGHT sample, then smoothed.

The four yields in the TT sample come from an extended maximum likelihood fit of

$$
\begin{aligned}
& N^{\mathbf{T T}} F^{\mathrm{obs}}\left(E_{\mathrm{T}, 1}^{\mathrm{iso}}, E_{\mathrm{T}, 2}^{\mathrm{iso}}\right) \\
& =N_{\gamma \gamma}^{\mathrm{TT}} F_{\gamma_{1}}\left(E_{\mathrm{T}, 1}^{\mathrm{iso}}\right) F_{\gamma_{2}}\left(E_{\mathrm{T}, 2}^{\mathrm{iso}}\right)+N_{\gamma \mathrm{j}}^{\mathrm{TT}} F_{\gamma_{1}}\left(E_{\mathrm{T}, 1}^{\mathrm{iso}}\right) F_{\mathrm{j}_{2}}\left(E_{\mathrm{T}, 2}^{\mathrm{iso}}\right) \\
& \quad+N_{\mathrm{j} \gamma}^{\mathrm{TT}} F_{\mathrm{j}_{1}}\left(E_{\mathrm{T}, 1}^{\mathrm{iso}}\right) F_{\gamma_{2}}\left(E_{\mathrm{T}, 2}^{\mathrm{iso}}\right)+N_{\mathrm{jj}}^{\mathrm{TT}} F_{\mathrm{jj}}\left(E_{\mathrm{T}, 1}^{\mathrm{iso}}, E_{\mathrm{T}, 2}^{\mathrm{iso}}\right) .
\end{aligned}
$$

Figure 4 shows the fit result for the full TT data set.
The yields in the TITI sample are evaluated by multiplying $N_{\gamma \gamma}^{\mathrm{TT}}$ by the integral of the 2-dimensional signal PDF in the region defined by $E_{\mathrm{T}, 1}^{\mathrm{iso}}<3 \mathrm{GeV}$ and $E_{\mathrm{T}, 2}^{\mathrm{iso}}<3 \mathrm{GeV}$. The procedure is applied to the events belonging to each


FIG. 4 (color online). Projections of the 2-dimensional PDF fit on transverse isolation energies of the two photon candidates: leading photon (top) and subleading photon (bottom). Solid circles represent the observed data. The continuous curve is the fit result, while the dashed-dotted curve shows the $\gamma \gamma$ component. The dashed line represents the background component of the leading and subleading photon sample, respectively.
bin of the observables $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$. The result is displayed in Fig. 3, by the open triangles.

The main sources of systematic uncertainties are (i) definition of the NONTIGHT control sample: ${ }_{-0 \%}^{+13 \%}$;
(ii) signal composition: $\pm 8 \%$; (iii) effect of material knowledge on signal: ${ }_{0 \%}^{+1.6 \%}$; (iv) signal PDF parameters: $\pm 0.7 \%$; (v) jet PDF parameters: $\pm 1.2 \%$; (vi) di-jet PDF parameters: $\pm 1 \%$; (vii) signal contamination in the NONTIGHT sample: ${ }_{0 \%}^{+1.2 \%}$. Effect (i) is estimated by changing the number of released strips cuts, as explained in Sec. VA. Effect (ii) has been estimated by artificially setting the fraction of fragmentation photons to $0 \%$ or to $100 \%$. Effect (iii) has been quantified by repeating the $e \rightarrow$ $\gamma$ extrapolation based on Monte Carlo samples with a distorted geometry. Effects (iv, v) have been estimated by randomly varying the parameters of the smoothing functions, within their covariance ellipsoid, and repeating the

2-dimensional fit. Effect (vi) has been estimated by randomly extracting a set of ( $\left.E_{\mathrm{T}, 1}^{\mathrm{iso}}, E_{\mathrm{T}, 2}^{\mathrm{iso}}\right)$ pairs, comparable to the experimental statistics, from the smoothed $F_{\mathrm{jj}} \mathrm{PDF}$, then resmoothing the obtained distribution and repeating the 2-dimensional fit. Effect (vii) has been estimated by taking the signal contamination from simulationneglected when computing the central value.

## 3. Isolation vs identification sideband counting (2D sidebands)

This method has been used in ATLAS in the inclusive photon cross-section measurement [10] and in the background decomposition in the search for the Higgs boson decaying into two photons [19].

The base di-photon sample must fulfil the selection with the strips cuts released, defined by the union of TIGHT and NONTIGHT samples and here referred to as LOOSE' $\left(\mathbf{L}^{\prime}\right)$. The leading photons in the $\mathbf{L}^{\prime} \mathbf{L}^{\prime}$ sample are divided into four categories $A, B, C, D$, depending on whether they satisfy the TIGHT selection and/or the isolation require-ment-see Fig. 5 (top). The signal region, defined by TIGHT and isolated photons (TI), contains $N_{A}$ candidates, whereas the three control regions contain $N_{B}, N_{C}, N_{D}$ candidates. Under the hypothesis that regions $B, C, D$ are largely dominated by background, and that the isolation energy of the background has little dependence on the TIGHT selection (as discussed in Sec. VA), the number of genuine leading photons $N_{A}^{\text {sig }}$ in region $A$, coming from $\gamma \gamma$ and $\gamma \mathrm{j}$ final states, can be computed [10] by solving the equation
$N_{A}^{\mathrm{sig}}=N_{A}-\left[\left(N_{B}-c_{1} N_{A}^{\mathrm{sig}}\right) \frac{N_{C}-c_{2} N_{A}^{\mathrm{sig}}}{N_{D}-c_{1} c_{2} N_{A}^{\mathrm{sig}}}\right] R^{\mathrm{bkg}}$.

Here, $c_{1}$ and $c_{2}$ are the signal fractions failing, respectively, the isolation requirement and the TIGHT selection. The former is computed from the isolation distributions, as extracted in Sec. VA; the latter is evaluated from Monte Carlo simulation, after applying the corrections to adapt it to the experimental shower shapes distributions [10]. The parameter $R^{\mathrm{bkg}}=\frac{N_{A}^{\mathrm{bkg}} N_{D}^{\mathrm{bkg}}}{N_{C}^{\mathrm{bg}} N_{B}^{\mathrm{kg}}}$ measures the degree of correlation between the isolation energy and the photon selection in the background: it is set to 1 to compute the central values, then varied according to the "di-jet-like" Monte Carlo prediction for systematic studies.

When the leading candidate is in the TI region, the subleading one is tested, and four categories $A^{\prime}, B^{\prime}, C^{\prime}$, $D^{\prime}$ are defined, as in the case of the leading candidate-see Fig. 5 (bottom). The number of genuine subleading photons $N_{A}^{\text {sig }}$, due to $\gamma \gamma$ and $\mathrm{j} \gamma$ final states, is computed by solving an equation analogous to (5).

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FIG. 5 (color online). Schematic representation of the twodimensional sideband method. The top plane displays the isolation ( x axis) and TIGHT identification (y axis) criteria for the classification of the leading photon candidate. When the leading photon belongs to region $A$, the same classification is applied to the subleading photon, as described by the bottom plane.
$N_{A}^{\text {sig }}$ and $N_{A}^{\prime}$ sig are related to the yields by

$$
N_{A}^{\mathrm{sig}}=\frac{N_{\gamma \gamma}^{\mathrm{TITI}}}{\epsilon^{\prime}}+\frac{N_{\gamma \mathrm{j}}^{\mathrm{TITI}}}{f^{\prime}}, \quad N_{A}^{\prime} \text { sig }=N_{\gamma \gamma}^{\mathrm{TITI}}+N_{\mathrm{j} \gamma}^{\mathrm{TITI}},
$$

where $\epsilon^{\prime}=\frac{1}{\left(1+c_{1}^{\prime}\right)\left(1+c_{2}^{\prime}\right)}$ is the probability that a subleading photon satisfies the TIGHT selection and isolation requirement, while $f^{\prime}$ is the analogous probability for a jet faking a subleading photon. The di-photon yield is therefore computed as

$$
\begin{equation*}
N_{\gamma \gamma}^{\mathrm{TITI}}=\frac{\epsilon^{\prime}\left(\alpha f^{\prime} N_{A}^{\mathrm{sig}}+(\alpha-1) N_{A}^{\prime \text { sig }}\right)}{(\alpha-1) \epsilon^{\prime}+\alpha f^{\prime}}, \tag{6}
\end{equation*}
$$

and $f^{\prime}$ can be computed from the observed quantities to be $f^{\prime}=\frac{N_{A}^{\prime}-N_{A}^{\text {Sisg }}}{N_{A}-N_{A}^{\text {sig }} / \epsilon^{\prime}}$. The parameter $\alpha$ is defined as the fraction of photon-jet events in which the jet fakes the leading photon, $\alpha=\frac{N_{i \gamma}^{\text {TITI }}}{N_{\gamma j}^{\text {TTI }}+N_{\text {ivT }}^{\text {TIT }}}$, whose value is taken from the PYTHIA photon-jet simulation.

The counts $N_{A}, N_{B}, N_{C}, N_{D}, N_{A}^{\prime}, N_{B}^{\prime}, N_{C}^{\prime}, N_{D}^{\prime}$, and hence the yield, can be computed for all events entering a given bin of $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$. The result is displayed in Fig. 3, by the open squares.

The main source of systematic error is the definition of the NONTIGHT sample: it induces an error of ${ }_{-10 \%}^{+7 \%}$. The other effects come from the uncertainties of the parameters entering Eq. (6). The main effects come from: (i) variation of $c_{1}^{\prime}: \pm 4 \%$; (ii) variation of $\alpha: \pm 3 \%$; (iii) variations of $R^{\mathrm{bkg}}, R^{\mathrm{bkg}}{ }_{-1.5 \%}^{+0 \%}$. The variations of $c_{1}, c_{2}, c_{2}^{\prime}$ have negligible impact.

## B. Electron background

Background from isolated electrons contaminates mostly the selected converted photon sample. The contamination in the di-photon analysis comes from several physical channels: (i) $e^{+} e^{-}$final states from Drell-Yan processes, $Z \rightarrow$ $e^{+} e^{-}$decay, $W^{+} W^{-} \rightarrow e^{+} e^{-} \nu \bar{\nu}$; (ii) $\gamma e^{ \pm}$final states from di-boson production, e.g. $\gamma W^{ \pm} \rightarrow \gamma e^{ \pm} \nu, \gamma Z \rightarrow \gamma e^{+} e^{-}$. The effect of the $Z \rightarrow e^{+} e^{-}$contamination is visible in Fig. 3 in the mass bin $80<m_{\gamma \gamma}<100 \mathrm{GeV}$.

Rather than quantifying each physical process separately, a global approach is chosen. The events reconstructed with $\gamma \gamma, \gamma e$, and $e e$ final states are counted, thus obtaining counts $N_{\gamma \gamma}, N_{\gamma e}$, and $N_{e e}$. Only photons and electrons satisfying a TIGHT selection and the calorimetric isolation $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$ are considered, and electrons are counted only if they are not reconstructed at the same time as photons. Such counts are related to the actual underlying yields $N_{\gamma \gamma}^{\text {true }}, N_{\gamma e}^{\text {tue }}, N_{e e}^{\text {tue }}$, defined as the number of reconstructed final states where both particles are correctly classified. Introducing the ratio $f_{e \rightarrow \gamma}=\frac{N_{e \rightarrow \gamma}}{N_{e \rightarrow e}}$ between genuine electrons that are wrongly and correctly classified, and likewise $f_{\gamma \rightarrow e}=\frac{N_{\gamma-e}}{N_{\gamma \gamma \gamma}}$ for genuine photons, the relationship between the $N$ and $N^{\text {true }}$ quantities is described by the following linear system:

$$
\left.\begin{array}{rl}
\left(\begin{array}{c}
N_{\gamma \gamma} \\
N_{\gamma e} \\
N_{e e}
\end{array}\right)= & \left(\begin{array}{ccc}
1 & f_{e \rightarrow \gamma} & \left(f_{e \rightarrow \gamma}\right)^{2} \\
2 f_{\gamma \rightarrow e} & \left(1+f_{e \rightarrow \gamma} f_{\gamma \rightarrow e}\right) & 2 f_{e \rightarrow \gamma} \\
\left(f_{\gamma \rightarrow e}\right)^{2} & f_{\gamma \rightarrow e} & 1
\end{array}\right) \\
& \times\left(\begin{array}{l}
N_{\gamma \gamma}^{\text {true }} \\
N_{\gamma e}^{\text {true }} \\
N_{e e}^{\text {true }}
\end{array}\right.
\end{array}\right)
$$

which can be solved for the unknown $N_{\gamma \gamma}^{\text {true }}$.

The value of $f_{e \rightarrow \gamma}$ is extracted from collision data, as $f_{e \rightarrow \gamma}=\frac{N_{\gamma e}}{2 N_{e e}}$, from events with an invariant mass within $\pm 5 \mathrm{GeV}$ of the $Z$ mass. The continuum background is removed using symmetric sidebands. The result is $f_{e \rightarrow \gamma}=$ $0.112 \pm 0.005$ (stat) $\pm 0.003$ (syst), where the systematic error comes from variations of the mass window and of the sidebands. This method has been tested on "di-jetlike" and $Z \rightarrow e^{+} e^{-}$Monte Carlo samples and shown to be unbiased. The value of $f_{\gamma \rightarrow e}$ is taken from the "di-jetlike" Monte Carlo: $f_{\gamma \rightarrow e}=0.0077$. To account for imperfect modelling, this value has also been set to 0 , or to 3 times the nominal value, and the resulting variations are considered as a source of systematic error.

The electron contamination is estimated for each bin of $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}$. and $\Delta \phi_{\gamma \gamma}$, and subtracted from the di-photon yield. The result, as a function of $m_{\gamma \gamma}$, is shown in Fig. 6. The fractional contamination as a function of $p_{\mathrm{T}, \gamma \gamma}$ and $\Delta \phi_{\gamma \gamma}$ is rather flat, amounting to $\sim 5 \%$.


FIG. 6 (color online). Electron background subtraction as a function of $m_{\gamma \gamma}$. The top plot displays the impurity, overall and for the $\gamma e$ and ee separately. The bottom plot shows the diphoton yield before (open squares) and after (solid circles) the electron background subtraction. The points are artificially shifted horizontally, to better display the different values.

## VII. EFFICIENCIES AND UNFOLDING

The signal is defined as a di-photon final state, which must satisfy precise kinematic cuts (referred to as "fiducial acceptance"'):
(i) both photons must have a transverse momentum $p_{\mathrm{T}}^{\gamma}>16 \mathrm{GeV}$ and must be in the pseudorapidity acceptance $\left|\eta^{\gamma}\right|<2.37$, with the exclusion of the region $1.37<\left|\eta^{\gamma}\right|<1.52$;
(ii) the separation between the two photons must be

$$
\Delta R_{\gamma \gamma}=\sqrt{\left(\eta_{1}^{\gamma}-\eta_{2}^{\gamma}\right)^{2}+\left(\phi_{1}^{\gamma}-\phi_{2}^{\gamma}\right)^{2}}>0.4
$$

(iii) both photons must be isolated, i.e. the transverse energy flow $E_{\mathrm{T}}^{\text {iso(part) }}$ due to interacting particles in a cone of angular radius $R<0.4$ must be $E_{\mathrm{T}}^{\text {iso(part) }}<$ 4 GeV .

These kinematic cuts define a phase space similar to the experimental selection described in Sec. III. In particular, the requirement on $E_{\mathrm{T}}^{\text {iso(part) }}$ has been introduced to match approximately the experimental cut on $E_{\mathrm{T}}^{\text {iso }}$. The value of $E_{\mathrm{T}}^{\text {iso(part) }}$ is corrected for the ambient energy, similarly to what is done for $E_{\mathrm{T}}^{\mathrm{iso}}$. From studies on a PYTHIA di-photon Monte Carlo sample, there is a high correlation between the two variables, and $E_{\mathrm{T}}^{\text {iso }}=3 \mathrm{GeV}$ corresponds to $E_{\mathrm{T}}^{\text {iso(part) }} \simeq 4 \mathrm{GeV}$.

A significant number of di-photon events lying outside the fiducial acceptance pass the experimental selection because of resolution effects: these are referred to as "below threshold" (BT) events.

The background subtraction provides the di-photon signal yields for events passing all selections (TITI). Such yields are called $N_{i}^{\text {TITI }}$, where the index $i$ flags the bins of the reconstructed observable $X^{\text {rec }}$ under consideration ( $X$ being $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$ ). The relationship between $N_{i}^{\text {TITI }}$ and the true yields $n_{\alpha}$ ( $\alpha$ being the bin index of the true value $X^{\text {true }}$ ) is:

$$
\begin{gather*}
N_{i}^{\mathrm{TITI}}=\epsilon^{\mathrm{trigger}} \epsilon_{i}^{\mathrm{TT}} N_{i}^{\mathrm{II}},  \tag{8}\\
N_{i}^{\mathrm{II}}\left(1-f_{i}^{B T}\right)=\sum_{\alpha} M_{i \alpha} \epsilon_{\alpha}^{R A} n_{\alpha}, \tag{9}
\end{gather*}
$$

where $N_{i}^{\mathrm{II}}$ is the number of reconstructed isolated diphoton events in the $i$ th bin, and
(i) $\epsilon^{\text {trigger }}$ is the trigger efficiency, computed for events where both photons satisfy the TIGHT identification and the calorimetric isolation;
(ii) $\epsilon_{i}^{\mathrm{TT}}$ is the efficiency of the TIGHT identification, for events where both photons satisfy the calorimetric isolation;
(iii) $f_{i}^{B T}$ is the fraction of "below-threshold" events;
(iv) $M_{i \alpha}$ is a "migration probability", i.e. the probability that an event with $X^{\text {true }}$ in bin- $\alpha$ is reconstructed with $X^{\text {rec }}$ in bin- $i$;
(v) $\epsilon_{\alpha}^{R A}$ accounts for both the reconstruction efficiency and the acceptance of the experimental cuts (kinematics and calorimetric isolation).

## A. Trigger efficiency

The trigger efficiency is computed from collision data, for events containing two reconstructed photons with transverse energy $E_{\mathrm{T}}^{\gamma}>16 \mathrm{GeV}$, both satisfying the TIGHT identification and the calorimetric isolation requirement (TITI). The computation is done in three steps.

First, a level-1 $e / \gamma$ trigger with an energy threshold of 5 GeV is studied: its efficiency, for reconstructed TI photons, is measured on an inclusive set of minimumbias events: for $E_{\mathrm{T}}^{\gamma}>16 \mathrm{GeV}$ it is $\epsilon_{0}=100.0_{-0.1}^{+0.0} \%-$ therefore such a trigger does not bias the sample. Next, a high-level photon trigger with a 15 GeV threshold is studied, for reconstructed TI photons selected by the level-1 trigger: its efficiency is $\epsilon_{1}=99.1_{-0.4}^{+0.3} \%$ for $E_{\mathrm{T}}^{\gamma}>$ 16 GeV . Finally, di-photon TITI events with the subleading photon selected by a high-level photon trigger are used to compute the efficiency of the di-photon 15 GeV threshold high-level trigger, obtaining $\epsilon_{2}=99.4_{-1.0}^{+0.5} \%$. The overall efficiency of the trigger is therefore $\epsilon^{\text {trigger }}=$ $\epsilon_{0} \epsilon_{1} \epsilon_{2}=\left(98.5_{-1.0}^{+0.6} \pm 1.0\right) \%$. The first uncertainty is statistical, the second is systematic and accounts for the contamination of photon-jet and di-jet events in the selected sample.

## B. Identification efficiency

The photon TIGHT identification efficiency $\epsilon^{\mathbf{T} \mid \mathbf{I}}$, for photon candidates satisfying the isolation cut $E_{\mathrm{T}}^{\text {iso }}<3 \mathrm{GeV}$, is computed as described in $\operatorname{Ref}$ [10], as a function of $\eta^{\gamma}$ and $E_{\mathrm{T}}^{\gamma}$. The efficiency is determined by applying the TIGHT selection to a Monte Carlo photon sample, where the shower shape variables have been shifted to better reproduce the observed distributions. The shift factors are obtained by comparing the shower shapes of photon candidates from a "di-jet-like" Monte Carlo sample to those observed in collision data. To enhance the photon component in the sample-otherwise overwhelmed by the jet background-only the photon candidates satisfying the TIGHT selection are considered. This procedure does not bias the bulk of the distribution under test appreciably, since the cuts have been tuned to reject only the tails of the photons' distributions. However, to check the systematic effect due to the selection, the shift factors are also recomputed applying the LOOSE selection.

Compared to Ref [10], the photon identification cuts have been reoptimized to reduce the systematic errors, and converted and unconverted photons treated separately. The photon identification efficiency is $\eta^{\gamma}$ dependent and increases with $E_{\mathrm{T}}^{\gamma}$, ranging from $\sim 60 \%$ for $16<E_{\mathrm{T}}^{\gamma}<$ 20 GeV to $\gtrsim 90 \%$ for $E_{\mathrm{T}}^{\gamma}>100 \mathrm{GeV}$. The overall systematic error is between $2 \%$ and $10 \%$, the higher values being
applicable at lower $E_{\mathrm{T}}^{\gamma}$ and for converted photons. The main sources of systematic uncertainty are (i) the systematic error on the shift factors; (ii) the knowledge of the detector material; (iii) the failure to detect a conversion, therefore applying the wrong TIGHT identification.

Rather than computing an event-level identification efficiency for each bin of each observable, the photon efficiency can be naturally accommodated into the event weights described in Sec. VI A 1, by dividing the weight $w^{(k)}$ of Eq. (4) by the product of the two photon efficiencies:

$$
\begin{equation*}
N_{i}^{\mathbf{I I}}=\sum_{k \in \operatorname{bin}-\mathrm{i}} \frac{w^{(k)}}{\left[\epsilon^{\mathbf{T} \mid \mathbf{I}}\left(\eta_{1}^{\gamma}, E_{\mathrm{T}}^{\gamma}\right) \epsilon^{\mathbf{T} \mid \mathbf{I}}\left(\eta_{2}^{\gamma}, E_{\mathrm{T}}^{2}{ }_{2}^{\gamma}\right)\right]^{(k)}}, \tag{10}
\end{equation*}
$$

where the sum is extended over all events in the TT sample and in the $i$ th bin. Here the identification efficiencies of the two photons are assumed to be uncorrelated-which is ensured by the separation cut $\Delta R>0.4$, and by the binning in $\eta^{\gamma}$ and $E_{\mathrm{T}}^{T}$.

The event efficiency, $\epsilon_{i}^{\mathrm{TT}}=\frac{N_{i}^{\text {TITI }}}{N_{i}^{\text {II }}}$, is essentially flat at $\sim 60 \%$ in $\Delta \phi_{\gamma \gamma}$, and increases with $m_{\gamma \gamma}$ and $p_{\mathrm{T}, \gamma \gamma}$, ranging from $\sim 55 \%$ to $\sim 80 \%$. Its total systematic error is $\sim 10 \%$, rather uniform over the $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$ ranges.

## C. Reconstruction, acceptance, isolation, and unfolding

The efficiency $\epsilon_{\alpha}^{R A}$ accounts for both the reconstruction efficiency and the acceptance of the experimental selection. It is computed for each bin of $X^{\text {true }}$, with Monte Carlo di-photon events generated with PYTHIA in the fiducial acceptance, as the fraction of events where both photons are reconstructed, pass the acceptance cuts and the calorimetric isolation. The value of $\epsilon_{\alpha}^{R A}$ ranges between $50 \%$ and $60 \%$. The two main sources of inefficiency are the local ECAL readout failures $(\sim-18 \%)$ and the calorimetric isolation ( $\sim-20 \%$ ).

The energy scale differences between Monte Carlo and collision data-calibrated on $Z \rightarrow e^{+} e^{-}$events-are taken into account. The uncertainties on the energy scale and resolution are propagated as systematic errors through the evaluation: the former gives an effect between $+3 \%$ and $-1 \%$ on the signal rate, while the latter has negligible impact.

In Monte Carlo, the calorimetric isolation energy, $E_{T}^{\text {iso }}$, needs to be corrected to match that observed in collision data. The correction is optimized on TIGHT photons, for which the background contamination can be removed (see Sec. VA), then it is applied to all photons in the Monte Carlo sample. The $E_{\mathrm{T}}^{\text {iso }}$ difference observed between Monte Carlo simulation and collision data may be entirely due to inaccurate GEANT4/detector modeling, or it can also be a consequence of the physical model in the generator (e.g. kinematics, fragmentation, hadronization). From the comparison between collision data and simulation, the two effects cannot be disentangled. To compute the central values of the results, the difference between simulation
and collision data is assumed to be entirely due to the detector simulation. As a cross-check, the opposite case is assumed: that the difference is entirely due to the generator model. In this case, the particle-level isolation $E_{\mathrm{T}}^{\text {iso(part) }}$ should also be corrected, using the $E_{\mathrm{T}}^{\text {iso(part) }} \rightarrow$ $E_{\mathrm{T}}^{\text {iso }}$ relationship described by the detector simulation. This modifies the definition of fiducial acceptance, and hence the values of $\epsilon_{\alpha}^{R A}$, resulting in a cross-section variation of $\sim-7 \%$, which is handled as an asymmetric systematic uncertainty.

The fraction of events "below threshold," $f_{i}^{B T}$, is computed from the same PYTHIA signal Monte Carlo sample,

TABLE I. Binned differential cross sections $d \sigma / d m_{\gamma \gamma}$, $d \sigma / d p_{\mathrm{T}, \gamma \gamma}, d \sigma / d \Delta \phi_{\gamma \gamma}$ for di-photon production. For each bin, the differential cross ection is quoted with its statistical and systematic uncertainties (symmetric and asymmetric, respectively). Values quoted as 0.000 are actually less than 0.0005 in absolute value.

| $\underline{m_{\gamma \gamma}[\mathrm{GeV}]}$ | $d \sigma / d m_{\gamma \gamma}[\mathrm{pb} / \mathrm{GeV}]$ |  |
| :---: | :---: | :---: |
| 0-30 | $0.20 \pm 0.05$ | ${ }_{-0.03}^{+0.05}$ |
| 30-40 | $1.8 \pm 0.3$ | +0.4 -0.3 |
| 40-50 | $2.3 \pm 0.3$ | ${ }_{-0.4}^{+0.6}$ |
| 50-60 | $1.83 \pm 0.24$ | ${ }_{-0.28}^{+0.36}$ |
| 60-70 | $0.74 \pm 0.17$ | ${ }_{-0.13}^{+0.19}$ |
| 70-80 | $0.45 \pm 0.15$ | ${ }_{-0.09}^{+0.11}$ |
| 80-100 | $0.40 \pm 0.06$ | ${ }_{-0.08}^{+0.08}$ |
| 100-150 | $0.079 \pm 0.022$ | ${ }_{-0.025}^{+0.025}$ |
| 150-200 | $0.026 \pm 0.009$ | ${ }_{-0.004}^{+0.006}$ |
| $\underline{p_{\text {T, } \gamma \gamma}[\mathrm{GeV}]}$ | $d \sigma / d p_{\text {T, } \gamma \gamma}[\mathrm{pb} / \mathrm{GeV}]$ |  |
| 0-10 | $4.5 \pm 0.4$ | ${ }_{-0.6}^{+0.9}$ |
| 10-20 | $2.2 \pm 0.3$ | ${ }_{-0.4}^{+0.5}$ |
| 20-30 | $0.94 \pm 0.22$ | ${ }_{-0.24}^{+0.28}$ |
| 30-40 | $0.62 \pm 0.16$ | ${ }_{-0.14}^{+0.21}$ |
| 40-50 | $0.26 \pm 0.10$ | +0.10 +0.09 |
| 50-60 | $0.36 \pm 0.09$ | ${ }_{-0.05}^{+0.09}$ |
| 60-80 | $0.06 \pm 0.03$ | ${ }_{-0.03}^{+0.03}$ |
| 80-100 | $0.048 \pm 0.019$ | ${ }_{-0.010}^{+0.009}$ |
| 100-150 | $0.003 \pm 0.004$ | ${ }_{-0.002}^{+0.003}$ |
| 150-200 | $0.000 \pm 0.002$ | $\begin{aligned} & +{ }_{-0.000}^{+0.000} \end{aligned}$ |
| $\Delta \phi_{\gamma \gamma}[\mathrm{rad}]$ | $d \sigma / d \Delta \phi_{\gamma \gamma}[\mathrm{pb} / \mathrm{rad}]$ |  |
| 0.00-1.00 | $4.9 \pm 1.1$ | ${ }_{-1.1}^{+1.5}$ |
| 1.00-2.00 | $8.9 \pm 1.8$ | ${ }_{-1.9}^{+2.5}$ |
| 2.00-2.50 | $24 \pm 4$ | ${ }_{-4}^{+6}$ |
| 2.50-2.80 | $56 \pm 8$ | +12 -9 |
| 2.80-3.00 | $121 \pm 13$ | ${ }_{-17}^{+24}$ |
| 3.00-3.14 | $173 \pm 16$ | $\begin{array}{r}+36 \\ -29 \\ \hline\end{array}$ |

for each bin of $X^{\text {rec }}$. Its value is maximum ( $\sim 12 \%$ ) for $m_{\gamma \gamma}$ about twice the $E_{\mathrm{T}}$ cut, and decreases to values $<5 \%$ for $m_{\gamma \gamma}>50 \mathrm{GeV}$.

The "migration matrix," $M_{i \alpha}$, is filled with PYTHIA Monte Carlo di-photon events in the fiducial acceptance, that are reconstructed, pass the acceptance cuts and the calorimetric isolation. The inversion of this matrix is
performed with an unfolding technique, based on Bayesian iterations [20]. The systematic uncertainties of the procedure have been estimated with a large number of toy data sets and found to be negligible. The result has also been tested to be independent of the initial ("prior") distributions. Moreover, it has been checked that a simpler bin-by-bin unfolding yields compatible results.

TABLE II. Breakdown of the total cross-section systematic uncertainty, for each bin of $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}$, and $\Delta \phi_{\gamma \gamma}$. The meaning of each column is as follows: " $\tilde{\mathbf{T}}$ " is the definition of the NONTIGHT control sample; " $\tilde{\mathbf{I}}$ " is the choice of the $E_{\mathrm{T}}^{\text {iso }}$ region used to normalize the NONTIGHT sample; "Matrix" refers to the statistical uncertainty of the matrix coefficients used by the event weighting; " $e \rightarrow \gamma$ " is the total systematic coming from the electron fake rate; "ID" is the overall uncertainty coming from the method used to derive the identification efficiency; "Material" is the effect of introducing a detector description with distorted material distribution; "Generator" shows the variation due to the usage of a different generator (SHERPA instead of PYTHIA); " $\sigma_{E}$ " and " $E$-scale" are due to uncertainties on energy resolution and scale; " $E_{\mathrm{T}}^{\mathrm{iso}(\text { part })}$ " is the effect of smearing the particle-level isolation $E_{\mathrm{T}}^{\text {iso(part) }}$; " $\int L d t$ " is the effect due to the total luminosity uncertainty. Values quoted as 0.000 are actually less than 0.0005 in absolute value.

| $m_{\gamma \gamma}[\mathrm{GeV}]$ | $\tilde{T}$ | $\tilde{\mathbf{I}}$ | Matrix | $e \rightarrow \gamma$ | ID | Material | Generator | $\sigma_{E}$ | $E$-scale | $E_{\mathrm{T}}^{\text {iso(part) }}$ | $\int L d t$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 0-30 | $\begin{aligned} & \hline+0.03 \\ & -0.01 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.005} \end{aligned}$ | $\begin{aligned} & +0.021 \\ & { }_{-0.022} \end{aligned}$ | $\begin{aligned} & +0.002 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.020 \\ & { }_{-0.017} \end{aligned}$ | $\begin{aligned} & \hline+0.021 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & \hline+0.03 \\ & -0.00 \end{aligned}$ | $\begin{aligned} & \hline+0.001 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.006 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & \hline-0.010 \end{aligned}$ | $\begin{aligned} & +0.007 \\ & { }_{-0.007} \end{aligned}$ |
| 30-40 | $\begin{aligned} & +0.17 \\ & { }_{-0.09} \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.05} \end{aligned}$ | $\begin{array}{r} +0.13 \\ { }_{-0.13} \end{array}$ | $\begin{aligned} & +0.008 \\ & -0.008 \end{aligned}$ | $\begin{aligned} & +0.22 \\ & { }_{-0.18} \end{aligned}$ | $\begin{aligned} & +0.3 \\ & { }_{-0.0} \end{aligned}$ | $\begin{aligned} & +0.014 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.003 \\ & -0.000 \end{aligned}$ | $\begin{array}{r} +0.04 \\ { }_{-0.03} \end{array}$ | $\begin{array}{r} +0.00 \\ { }_{-0.09} \end{array}$ | $\begin{array}{r} +0.06 \\ { }_{-0.06} \end{array}$ |
| 40-50 | $\begin{aligned} & +0.3 \\ & -0.1 \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.06} \end{aligned}$ | $\begin{array}{r} +0.19 \\ -0.19 \\ -0.19 \end{array}$ | $\begin{aligned} & +0.008 \\ & -0.008 \end{aligned}$ | $\begin{aligned} & +0.24 \\ & { }_{-0.20} \end{aligned}$ | $\begin{aligned} & +0.3 \\ & -0.0 \end{aligned}$ | $\begin{array}{r} +0.11 \\ { }_{-0.00} \end{array}$ | $\begin{aligned} & +0.024 \\ & -0.000 \end{aligned}$ | $\begin{array}{r} +0.09 \\ { }_{-0.03} \end{array}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.17} \end{aligned}$ | $\begin{aligned} & +0.08 \\ & { }_{-0.08} \end{aligned}$ |
| 50-60 | $\begin{aligned} & +0.20 \\ & -0.13 \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.04} \end{aligned}$ | $\begin{array}{r} +0.14 \\ -0.14 \end{array}$ | $\begin{aligned} & +0.007 \\ & -0.007 \end{aligned}$ | $\begin{aligned} & +0.15 \\ & { }_{-0.13} \end{aligned}$ | $\begin{array}{r} +0.19 \\ { }_{-0.00} \end{array}$ | $\begin{aligned} & +0.05 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.003 \\ & { }_{-0.000} \end{aligned}$ | $\begin{aligned} & +0.06 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.13} \end{aligned}$ | $\begin{aligned} & +0.06 \\ & { }_{-0.06} \end{aligned}$ |
| 60-70 | $\begin{aligned} & +0.14 \\ & { }_{-0.06} \end{aligned}$ | $\begin{aligned} & +0.001 \\ & { }_{-0.016} \end{aligned}$ | $\begin{array}{r} +0.09 \\ { }_{-0.09} \end{array}$ | $\begin{aligned} & +0.004 \\ & -0.004 \end{aligned}$ | $\begin{aligned} & +0.05 \\ & { }_{-0.04} \end{aligned}$ | $\begin{aligned} & +0.07 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.04 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.007 \\ & { }_{-0.000} \end{aligned}$ | $\begin{array}{r} +0.03 \\ { }_{-0.02} \end{array}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.05} \end{aligned}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.03} \end{aligned}$ |
| 70-80 | $\begin{aligned} & +0.06 \\ & { }_{-0.06} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.007} \end{aligned}$ | $\begin{array}{r} +0.05 \\ { }_{-0.06} \end{array}$ | $\begin{aligned} & +0.003 \\ & -0.003 \end{aligned}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.07 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.002 \\ & -0.001 \end{aligned}$ | $\begin{array}{r} +0.009 \\ -0.002 \end{array}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.015 \\ & { }_{-0.015} \end{aligned}$ |
| 80-100 | $\begin{aligned} & +0.04 \\ & { }_{-0.05} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.005} \end{aligned}$ | $\begin{array}{r} +0.04 \\ { }_{-0.04} \end{array}$ | $\begin{array}{r} +0.019 \\ -0.019 \end{array}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.02} \end{aligned}$ | $\begin{array}{r} +0.04 \\ { }_{-0.00} \end{array}$ | $\begin{array}{r} +0.012 \\ -0.000 \end{array}$ | $\begin{aligned} & +0.004 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.013 \\ & -0.003 \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.013 \\ & -0.013 \end{aligned}$ |
| 100-150 | $\begin{array}{r} +0.019 \\ { }_{-0.016} \end{array}$ | $\begin{aligned} & +0.001 \\ & { }_{-0.001} \end{aligned}$ | $\begin{aligned} & +0.015 \\ & { }_{-0.018} \end{aligned}$ | $\begin{array}{r} +0.001 \\ { }_{-0.001} \end{array}$ | $\begin{aligned} & +0.004 \\ & -0.003 \end{aligned}$ | $\begin{aligned} & +0.002 \\ & -0.001 \end{aligned}$ | $\begin{aligned} & +0.004 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.001} \end{aligned}$ | $\begin{aligned} & +0.002 \\ & -0.003 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.005 \end{aligned}$ | $\begin{aligned} & +0.003 \\ & -0.003 \end{aligned}$ |
| 150-200 | $\begin{aligned} & +0.002 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ | $\begin{array}{r} +0.003 \\ -0.003 \end{array}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.002 \\ & { }_{-0.001} \end{aligned}$ | $\begin{array}{r} +0.004 \\ -0.000 \end{array}$ | $\begin{aligned} & +0.001 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.001 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.001 \\ & { }_{-0.001} \end{aligned}$ |
| $p_{\mathrm{T}, \gamma \gamma}[\mathrm{GeV}]$ | $\tilde{\mathbf{T}}$ | I | matrix | $e \rightarrow \gamma$ | ID | material | generator | $\sigma_{E}$ | $E$-scale | $E_{\mathrm{T}}^{\mathrm{iso}(\text { part })}$ | $\int L d t$ |
| 0-10 | $\begin{aligned} & \hline+0.3 \\ & -0.2 \end{aligned}$ | $\begin{aligned} & \hline+0.00 \\ & -0.09 \\ & -0 . \end{aligned}$ | $\begin{aligned} & \hline+0.3 \\ & -0.3 \end{aligned}$ | $\begin{aligned} & \hline+0.03 \\ & -0.03 \end{aligned}$ | $\begin{aligned} & \hline+0.4 \\ & -0.4 \end{aligned}$ | $\begin{aligned} & \hline+0.6 \\ & -0.0 \end{aligned}$ | $\begin{aligned} & +0.10 \\ & -0.00 \\ & \end{aligned}$ | $\begin{aligned} & \hline+0.03 \\ & -0.00 \end{aligned}$ | $\begin{aligned} & \hline+0.12 \\ & -0.05 \end{aligned}$ | $\begin{aligned} & +0.0 \\ & -0.3 \end{aligned}$ | $\begin{aligned} & \hline+0.15 \\ & -0.15 \end{aligned}$ |
| 10-20 | $\begin{aligned} & +0.3 \\ & { }_{-0.2} \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.05} \end{aligned}$ | $\begin{aligned} & +0.21 \\ & { }_{-0.22} \end{aligned}$ | $\begin{aligned} & +0.015 \\ & -0.015 \end{aligned}$ | $\begin{array}{r} +0.20 \\ { }_{-0.17} \end{array}$ | $\begin{aligned} & +0.21 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.11 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.001 \\ & { }_{-0.001} \end{aligned}$ | $\begin{aligned} & +0.06 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.15} \end{aligned}$ | $\begin{aligned} & +0.08 \\ & { }_{-0.08} \end{aligned}$ |
| 20-30 | $\begin{aligned} & +0.21 \\ & { }_{-0.16} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.025} \end{aligned}$ | $\begin{array}{r} +0.13 \\ -0.14 \end{array}$ | $\begin{aligned} & +0.008 \\ & -0.008 \end{aligned}$ | $\begin{array}{r} +0.07 \\ { }_{-0.06} \end{array}$ | $\begin{aligned} & +0.10 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.022 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.010 \\ & { }_{-0.000} \end{aligned}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.02} \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.08} \end{aligned}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.03} \end{aligned}$ |
| 30-40 | $\begin{array}{r} +0.13 \\ { }_{-0.08} \end{array}$ | $\begin{array}{r} +0.000 \\ -0.012 \end{array}$ | $\begin{array}{r} +0.09 \\ { }_{-0.10} \end{array}$ | $\begin{aligned} & +0.006 \\ & { }_{-0.006} \end{aligned}$ | $\begin{aligned} & +0.06 \\ & { }_{-0.05} \end{aligned}$ | $\begin{aligned} & +0.11 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.08 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.007 \\ & { }_{-0.000} \end{aligned}$ | $\begin{array}{r} +0.015 \\ { }_{-0.009}^{+0 .} \end{array}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.03} \end{aligned}$ | $\begin{array}{r} +0.021 \\ -0.021 \end{array}$ |
| 40-50 | $\begin{aligned} & +0.08 \\ & { }_{-0.06} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.007} \end{aligned}$ | $\begin{aligned} & +0.05 \\ & { }_{-0.06} \end{aligned}$ | $\begin{aligned} & +0.004 \\ & -0.004 \end{aligned}$ | $\begin{aligned} & +0.018 \\ & -0.017 \end{aligned}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.005 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.012} \end{aligned}$ | $\begin{aligned} & +0.00 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.015 \end{aligned}$ | $\begin{aligned} & +0.009 \\ & -0.009 \end{aligned}$ |
| 50-60 | $\begin{aligned} & +0.03 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.007} \end{aligned}$ | $\begin{aligned} & +0.02 \\ & { }_{-0.03} \end{aligned}$ | $\begin{aligned} & +0.006 \\ & { }_{-0.006} \end{aligned}$ | $\begin{aligned} & +0.03 \\ & { }_{-0.02} \end{aligned}$ | $\begin{aligned} & +0.04 \\ & { }_{-0.00} \end{aligned}$ | $\begin{array}{r} +0.04 \\ { }_{-0.00} \end{array}$ | $\begin{aligned} & +0.013 \\ & -0.000 \end{aligned}$ | $\begin{array}{r} +0.05 \\ { }_{-0.01} \end{array}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.023} \end{aligned}$ | $\begin{aligned} & +0.012 \\ & -0.012 \end{aligned}$ |
| 60-80 | $\begin{aligned} & +0.021 \\ & -0.023 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.001} \end{aligned}$ | $\begin{aligned} & +0.014 \\ & { }_{-0.016} \end{aligned}$ | $\begin{array}{r} +0.001 \\ -0.001 \end{array}$ | $\begin{aligned} & +0.003 \\ & -0.003 \end{aligned}$ | $\begin{aligned} & +0.005 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.004 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.001 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.004 \end{aligned}$ | $\begin{aligned} & +0.002 \\ & -0.002 \end{aligned}$ |
| 80-100 | $\begin{aligned} & +0.006 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.001} \end{aligned}$ | $\begin{array}{r} +0.005 \\ -0.005 \end{array}$ | $\begin{aligned} & +0.002 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.003 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.002 \\ & -0.006 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.005} \end{aligned}$ | $\begin{array}{r} +0.001 \\ -0.000 \end{array}$ | $\begin{aligned} & +0.004 \\ & -0.001 \end{aligned}$ | $\begin{array}{r} +0.000 \\ -0.004 \end{array}$ | $\begin{aligned} & +0.002 \\ & -0.002 \end{aligned}$ |
| 100-150 | $\begin{aligned} & +0.002 \\ & -0.001 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ | $\begin{aligned} & +0.001 \\ & -0.002 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.001 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ |
| 150-200 | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ | $\begin{array}{r} +0.000 \\ { }_{-0.000} \end{array}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.000} \end{aligned}$ | $\begin{array}{r} +0.000 \\ -0.000 \end{array}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ | $\begin{array}{r} +0.000 \\ -0.000 \end{array}$ | $\begin{aligned} & +0.000 \\ & -0.000 \end{aligned}$ |
| $\Delta \phi_{\gamma \gamma}[\mathrm{rad}]$ | $\widetilde{T}$ | $\tilde{\mathbf{I}}$ | matrix | $e \rightarrow \gamma$ | ID | material | generator | $\sigma_{E}$ | $E$-scale | $E_{\mathrm{T}}^{\mathrm{iso}(\text { part })}$ | $\int L d t$ |
| 0.00-1.00 | $\begin{aligned} & +1.1 \\ & -0.5 \end{aligned}$ | $\begin{aligned} & \hline+0.00 \\ & -0.14 \end{aligned}$ | $\begin{aligned} & +0.8 \\ & -0.8 \end{aligned}$ | $\begin{aligned} & \hline+0.05 \\ & { }_{-0.05} \end{aligned}$ | $\begin{aligned} & +0.4 \\ & -0.4 \end{aligned}$ | $\begin{aligned} & +0.4 \\ & -0.0 \end{aligned}$ | $\begin{aligned} & +0.3 \\ & -0.0 \end{aligned}$ | $\begin{aligned} & +0.000 \\ & { }_{-0.017} \end{aligned}$ | $\begin{aligned} & \hline+0.14 \\ & -0.08 \end{aligned}$ | $\begin{aligned} & +0.0 \\ & { }_{-0.3} \end{aligned}$ | $\begin{aligned} & \hline+0.17 \\ & { }_{-0.17} \end{aligned}$ |
| 1.00-2.00 | $\begin{array}{r} +1.6 \\ -1.0 \end{array}$ | $\begin{aligned} & +0.0 \\ & { }_{-0.3} \end{aligned}$ | $\begin{aligned} & +1.2 \\ & -1.2 \end{aligned}$ | $\begin{array}{r} +0.07 \\ { }_{-0.07} \end{array}$ | $\begin{aligned} & +0.8 \\ & { }_{-0.7} \end{aligned}$ | $\begin{aligned} & +1.0 \\ & { }_{-0.0} \end{aligned}$ | $\begin{aligned} & +0.5 \\ & -0.0 \end{aligned}$ | $\begin{aligned} & +0.023 \\ & -0.000 \end{aligned}$ | $\begin{aligned} & +0.23 \\ & { }_{-0.10} \end{aligned}$ | $\begin{aligned} & +0.0 \\ & { }_{-0.5} \end{aligned}$ | $\begin{aligned} & +0.3 \\ & -0.3 \end{aligned}$ |
| 2.00-2.50 | $\begin{aligned} & +3 \\ & -2 \end{aligned}$ | $\begin{aligned} & +0.0 \\ & { }_{-0.4} \end{aligned}$ | $\begin{aligned} & +2.2 \\ & -2.3 \end{aligned}$ | $\begin{array}{r} +0.17 \\ { }_{-0.17} \end{array}$ | $\begin{aligned} & +2.2 \\ & -1.8 \end{aligned}$ | $\begin{aligned} & +3 \\ & -0 \end{aligned}$ | $\begin{aligned} & +1.5 \\ & -0.0 \end{aligned}$ | $\begin{aligned} & +0.10 \\ & { }_{-0.00} \end{aligned}$ | $\begin{aligned} & +0.6 \\ & -0.4 \end{aligned}$ | $\begin{aligned} & +0.0 \\ & -1.3 \end{aligned}$ | $\begin{aligned} & +0.8 \\ & -0.8 \end{aligned}$ |
| 2.50-2.80 | $\begin{aligned} & +6 \\ & { }_{-5} \end{aligned}$ | $\begin{aligned} & +0.0 \\ & -1.3 \end{aligned}$ | $\begin{aligned} & +5 \\ & -5 \end{aligned}$ | $\begin{aligned} & +0.4 \\ & -0.4 \end{aligned}$ | $\begin{array}{r} +5 \\ -4 \end{array}$ | $\begin{aligned} & +6 \\ & -0 \end{aligned}$ | $\begin{aligned} & +0.3 \\ & { }_{-0.0} \end{aligned}$ | $\begin{aligned} & +0.4 \\ & { }_{-0.0} \end{aligned}$ | $\begin{array}{r} +1.8 \\ -1.0 \end{array}$ | $\begin{aligned} & +0 \\ & -4 \end{aligned}$ | $\begin{array}{r} +1.9 \\ -1.9 \end{array}$ |
| 2.80-3.00 | $\begin{gathered} +11 \\ { }_{-5} \end{gathered}$ | $\begin{aligned} & +0 \\ & -3 \end{aligned}$ | $\begin{gathered} +9 \\ -10 \end{gathered}$ | $\begin{aligned} & +0.9 \\ & -0.9 \end{aligned}$ | $\begin{gathered} +11 \\ +-9 \end{gathered}$ | $\begin{gathered} +14 \\ { }_{-0} \end{gathered}$ | $\begin{aligned} & +2.3 \\ & -0.0 \end{aligned}$ | $\begin{aligned} & +0.7 \\ & { }_{-0.0} \end{aligned}$ | $\begin{aligned} & +4 \\ & -1 \end{aligned}$ | $\begin{array}{r} +0 \\ -9 \end{array}$ | $\begin{aligned} & +4 \\ & -4 \end{aligned}$ |
| 3.00-3.14 | $\begin{array}{r} +19 \\ +16 \\ \hline \hline \end{array}$ | $\begin{array}{r} +0 \\ +0 \\ \hline \\ \hline \end{array}$ | $\begin{array}{r} +14 \\ +15 \\ \hline \hline \end{array}$ | $\begin{array}{r} +1.5 \\ -1.5 \\ \hline \hline \end{array}$ | $\begin{array}{r} +16 \\ -13 \\ \hline \hline \end{array}$ | $\begin{gathered} +18 \\ -0 \\ \hline \hline \end{gathered}$ | $\begin{array}{r} +9 \\ +0 \\ \hline-0 \\ \hline \hline \end{array}$ | $\begin{array}{r} +0.6 \\ +0.0 \\ \hline \hline \end{array}$ | $\begin{array}{r} +4 \\ -2 \\ \hline \end{array}$ | $\begin{array}{r} +0 \\ -12 \\ \hline \hline \end{array}$ | ${ }_{-6}^{+6}$ |

As the evaluation of $\epsilon_{\alpha}^{R A}, f_{i}^{B T}, M_{i \alpha}$ may strongly depend on the simulation modeling, two additional Monte Carlo samples have been used, the first with more material modeled in front of the calorimeter, and the second with a different generator (SHERPA): the differences on the computed signal rates are $\sim+10 \%$ and $\lesssim+5 \%$ respectively, and are treated as systematic errors.

## VIII. CROSS-SECTION MEASUREMENT

The di-photon production cross section is evaluated from the corrected binned yields $n_{\alpha}$, divided by the integrated luminosity $\int L d t=(37.2 \pm 1.3) \mathrm{pb}^{-1}$ [8]. The results are presented as differential cross sections, as functions of the three observables $m_{\gamma \gamma}, p_{\mathrm{T}, \gamma \gamma}, \Delta \phi_{\gamma \gamma}$, for a phase space defined by the fiducial acceptance cuts in Sec. VII. In Table I, the differential cross section is quoted for each bin, with its statistical and systematic uncertainty. In Table II, all the considered sources of systematic errors are listed separately.

The experimental measurement is compared with theoretical predictions from the DIPHOX [21] and ResBos [22] NLO generators in Figs. 7-9. The DIPHOX and ResBos evaluation has been carried out using the NLO fragmentation function [23] and the CTEQ6.6 parton density function


FIG. 7 (color online). Differential cross-section $d \sigma / d m_{\gamma \gamma}$ of diphoton production. The solid circles display the experimental values, the hatched bands display the NLO computations by DIPHOX and ResBos. The bottom panels show the relative difference between the measurements and the NLO predictions. The data/ theory point in the bin $0<m_{\gamma \gamma}<30 \mathrm{GeV}$ lies above the frames.


FIG. 8 (color online). Differential cross-section $d \sigma / d p_{\mathrm{T}, \gamma \gamma}$ of di-photon production. The solid circles display the experimental values, the hatched bands display the NLO computations by DIPHOX and ResBos. The bottom panels show the relative difference between the measurements and the NLO predictions. The data point in the bin $150<p_{\mathrm{T}, \gamma \gamma}<200 \mathrm{GeV}$ in the main panel lies below the frame.
(PDF) set [24]. The fragmentation, normalization and factorization scales are set equal to $m_{\gamma \gamma}$. The same fiducial acceptance cuts introduced in the signal definition (Sec. VII) are applied. Since neither generator models the hadronization, it is not possible to apply a requirement on $E_{\mathrm{T}}^{\text {iso(part) }}$ : the closest isolation variable available in such generators is the "partonic isolation," which is therefore required to be less then 4 GeV . The computed cross section shows a weak dependence on the partonic isolation cut: moving it to 2 or 6 GeV produces variations within $5 \%$, smaller than the theoretical systematic errors.

The theory uncertainty error bands come from scale and PDF uncertainties evaluated from DIPHOX: (i) variation of renormalization, fragmentation, and factorization scales: each is varied to $\frac{1}{2} m_{\gamma \gamma}$ and $2 m_{\gamma \gamma}$, and the envelope of all variations is assumed as a systematic error; (ii) variation of the eigenvalues of the PDFs: each is varied by $\pm 1 \sigma$, and positive/negative variations are summed in quadrature separately. As an alternative, the MSTW 2008 PDF set has been used: the difference with respect to CTEQ6.6 is an overall increase by $\sim 10 \%$, which is covered by the CTEQ6.6 total systematic error.

The measured distribution of $d \sigma / d \Delta \phi_{\gamma \gamma}$ (Fig. 9) is clearly broader than the DIPHOX and ResBos predictions:


FIG. 9 (color online). Differential cross-section $d \sigma / d \Delta \phi_{\gamma \gamma}$ of di-photon production. The solid circles display the experimental values, the hatched bands display the NLO computations by DIPHOX and ResBos. The bottom panels show the relative difference between the measurements and the NLO predictions.
more photon pairs are seen in data at low $\Delta \phi_{\gamma \gamma}$ values, while the theoretical predictions favor a larger back-toback production ( $\Delta \phi_{\gamma \gamma} \simeq \pi$ ). This result is qualitatively in agreement with previous measurements at the Tevatron [5,6]. The distribution of $d \sigma / d m_{\gamma \gamma}$ (Fig. 7) agrees within the assigned uncertainties with both the DIPHOX and ResBos predictions, apart from the region $m_{\gamma \gamma}<2 E_{\mathrm{T}}^{\text {cut }}$ ( $E_{\mathrm{T}}^{\mathrm{cut}}=16 \mathrm{GeV}$ being the applied cut on the photon transverse momenta): as this region is populated by events with small $\Delta \phi_{\gamma \gamma}$, the poor quality of the predictions can be related to the discrepancy observed in the $\Delta \phi_{\gamma \gamma}$ distribution. The result for $d \sigma / d p_{\mathrm{T}, \gamma \gamma}$ (Fig. 8) is in agreement with both DIPHOX and ResBos: the maximum deviation, about $2 \sigma$, is observed in the region $50<p_{\mathrm{T}, \gamma \gamma}<60 \mathrm{GeV}$.

## IX. CONCLUSIONS

This paper describes the measurement of the production cross section of isolated di-photon final states in protonproton collisions, at a center-of-mass energy $\sqrt{s}=7 \mathrm{TeV}$, with the ATLAS experiment. The full data sample collected in 2010, corresponding to an integrated luminosity of $37.2 \pm 1.3 \mathrm{pb}^{-1}$, has been analyzed.

The selected sample consists of 2022 candidate events containing two reconstructed photons, with transverse
momenta $p_{\mathrm{T}}>16 \mathrm{GeV}$ and satisfying tight identification and isolation requirements. All the background sources have been investigated with data-driven techniques and subtracted. The main background source, due to hadronic jets in photon-jet and di-jet events, has been estimated with three computationally independent analyses, all based on shower shape variables and isolation, which give compatible results. The background due to isolated electrons from $W$ and $Z$ decays is estimated with collision data, from the proportions of observed $e e, \gamma e$, and $\gamma \gamma$ final states, in the $Z$-mass region and elsewhere.
The result is presented in terms of differential cross sections as functions of three observables: the invariant mass $m_{\gamma \gamma}$, the total transverse momentum $p_{\mathrm{T}, \gamma \gamma}$, and the azimuthal separation $\Delta \phi_{\gamma \gamma}$ of the photon pair. The experimental results are compared with NLO predictions obtained with DIPHOX and ResBos generators. The observed spectrum of $d \sigma / d \Delta \phi_{\gamma \gamma}$ is broader than the NLO predictions. The distribution of $d \sigma / d m_{\gamma \gamma}$ is in good agreement with both the DIPHOX and ResBos predictions, apart from the low mass region. The result for $d \sigma / d p_{\mathrm{T}, \gamma \gamma}$ is generally well described by DIPHOX and ResBos.

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# Search for Diphoton Events with Large Missing Transverse Energy in 7 TeV Proton-Proton Collisions with the ATLAS Detector 

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#### Abstract

A search for diphoton events with large missing transverse energy is presented. The data were collected with the ATLAS detector in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ at the CERN Large Hadron Collider and correspond to an integrated luminosity of $3.1 \mathrm{pb}^{-1}$. No excess of such events is observed above the standard model background prediction. In the context of a specific model with one universal extra dimension with compactification radius $R$ and gravity-induced decays, values of $1 / R<729 \mathrm{GeV}$ are excluded at $95 \%$ C. L., providing the most sensitive limit on this model to date.


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In the standard model (SM), the production in protonproton $(p p)$ collisions of diphoton $(\gamma \gamma)$ events with large missing transverse energy $\left(E_{T}^{\text {miss }}\right)$ is mainly due to $W / Z+$ $\gamma \gamma$ processes. Taking into account the branching ratios of $W / Z$ decays including at least one neutrino, the cross sections are only a few femtobarns for $7 \mathrm{TeV} p p$ collisions. In contrast, some new physics models predict much larger $\gamma \gamma+E_{T}^{\text {miss }}$ rates. This Letter reports the first $\gamma \gamma+E_{T}^{\text {miss }}$ search with LHC data, using data recorded with the ATLAS detector. The results are interpreted in the context of a universal extra dimension (UED) model.

UED models [1] postulate the existence of additional spatial dimensions in which all SM particles can propagate, leading to the existence for each SM particle of a series of excitations, known as a Kaluza-Klein (KK) tower. This analysis considers the case of a single $\mathrm{TeV}^{-1}$-sized UED, with compactification radius $R$. The masses of the states of successive levels in the tower are separated by $\approx 1 / R$. For a given KK level, the approximate mass degeneracy of the KK excitations is broken by radiative corrections [2]. The lightest KK particle (LKP) is the KK photon of the first level, denoted $\gamma^{*}$. At the LHC, the main UED process would be production via the strong interaction of a pair of first-level KK quarks and/or gluons [3], which would decay via cascades involving other KK particles until reaching the LKP at the end of the decay chain. If the UED model is embedded in a larger space with $N$ additional $\mathrm{eV}^{-1}$-sized dimensions accessible only to gravity [4], the LKP could decay gravitationally via $\gamma^{*} \rightarrow \gamma+G$ [5], where $G$ represents one of a tower of eV-spaced graviton states. With two decay chains per event, the final state would be $\gamma \gamma+E_{T}^{\text {miss }}+X$, where $E_{T}^{\text {miss }}$ results from

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the escaping gravitons and $X$ represents SM particles emitted in the cascade decays.

The UED model considered is defined by specifying $R$ and $\Lambda$, the ultraviolet cutoff used in the calculation of radiative corrections to the KK masses. This analysis treats $R$ as a free parameter and, following the theory calculations [2], sets $\Lambda$ such that $\Lambda R=20$. For $1 / R=700 \mathrm{GeV}$, the masses of the first-level KK photon, quark, and gluon are 700,815 , and 865 GeV , respectively [6]. The $\gamma^{*}$ mass is insensitive to $\Lambda$, while other KK masses change by typically a few percent when varying $\Lambda R$ in the range 10-30. The gravitational decay widths of the KK particles are set by $N$ and $M_{D}$, the Planck scale in the $(4+N)$-dimensional theory. For the chosen values of $N=6$ and $M_{D}=5 \mathrm{TeV}$, and provided $1 / R<1 \mathrm{TeV}$, the LKP is the only KK particle to have an appreciable rate of gravitational decay. The same parameter values were used in the only previous study of this model, in which the D0 experiment excluded at $95 \% \mathrm{C}$. L. values of $1 / R<477 \mathrm{GeV}$ [7].

Monte Carlo (MC) signal samples were produced for a range of $1 / R$ values using the implementation [6] of the UED model in PYTHIA [8] version 6.421, and using the MC09 parameter tune [9]. The MC samples were processed through the ATLAS detector simulation [10] based on GEANT4 [11]. In addition to the two high transverse energy $\left(E_{T}\right)$ photons and large $E_{T}^{\text {miss }}$, the signal events typically include several high- $E_{T}$ jets due to the cascade decays, with the $E_{T}$ spectrum of the leading jet peaking at $\approx 100 \mathrm{GeV}$ for $1 / R=700 \mathrm{GeV}$.

The ATLAS detector [12] is a multipurpose particle physics apparatus with a forward-backward symmetric cylindrical geometry and nearly $4 \pi$ solid angle coverage. ATLAS uses a Cartesian right-handed coordinate system, with the nominal collision point at the origin. The anticlockwise beam direction defines the positive $z$ axis, while the positive $x$ axis points from the collision point to the center of the LHC ring and the positive $y$ axis points upward. The angles $\phi$ and $\theta$ are the azimuthal and polar angles. The pseudorapidity is defined as
$\eta=-\ln [\tan (\theta / 2)]$. Closest to the beam line are tracking detectors which use layers of silicon-based and straw-tube detectors, located inside a thin superconducting solenoid that provides a 2 T magnetic field, to measure the trajectories of charged particles. The solenoid is surrounded by a hermetic calorimeter system. A liquid-argon (LAr) sampling calorimeter is divided into a central barrel calorimeter and two end-cap calorimeters, each housed in a separate cryostat. Fine-grained LAr electromagnetic (EM) calorimeters, with excellent energy resolution, provide coverage for $|\eta|<3.2$. In the region $|\eta|<2.5$, the EM calorimeters are segmented into three longitudinal layers and the second layer, in which most of the EM shower energy is deposited, is divided into cells of granularity of $\Delta \eta \times \Delta \phi=0.025 \times$ 0.025. A presampler, covering $|\eta|<1.8$, is used to correct for energy lost upstream of the calorimeter. An ironscintillator tile calorimeter provides hadronic coverage in the range $|\eta|<1.7$. In the end caps $(|\eta|>1.5)$, LAr hadronic calorimeters match the outer $|\eta|$ limits of the end-cap EM calorimeters. LAr forward calorimeters provide both EM and hadronic energy measurements, and extend the coverage to $|\eta|<4.9$. Outside the calorimeters is an extensive muon system including large superconducting toroidal magnets.

The reconstruction of photons is described in detail in Ref. [13]. To select photon candidates, EM calorimeter clusters were required to pass several quality criteria and to lie outside problematic calorimeter regions. Photon candidates were required to have $|\eta|<1.81$ and to be outside the transition region $1.37<|\eta|<1.52$ between the barrel and the end-cap calorimeters. The analysis uses a "loose" photon selection, which includes cuts on the energy in the hadronic calorimeter as well as on variables that require the transverse width of the shower, measured in the second EM calorimeter layer, be consistent with the narrow width expected for an EM shower. The loose selection provides a high photon efficiency with modest rejection against the background from jets.

The reconstruction of $E_{T}^{\text {miss }}$ is based on topological calorimeter clusters [14] with $|\eta|<4.5$ that are seeded by any cell with energy higher than 4 times its noise level. In an iterative procedure, the cluster grows by including all neighboring cells with energy higher than twice the noise, plus all cells neighboring the boundary of this three-dimensional collection. Each cluster is classified as EM or hadronic, depending on its topology, and the cluster energy is calibrated to correct for the noncompensating calorimeter response, energy losses in dead material, and out-of-cluster energies. Events reconstructed with large $E_{T}^{\text {miss }}$ were studied in detail with early data [15]. Rare background events with large transverse energies, unrelated to the collision and concentrated in a few cells, due mainly to discharges and noise, have been observed. Cuts were applied to eliminate such backgrounds, rejecting less than $0.05 \%$ of the selected events while having a negligible impact on the signal efficiency.

The data sample was collected during stable beam periods of $7 \mathrm{TeV} p p$ collisions at the LHC, and corresponds to an integrated luminosity of $3.1 \mathrm{pb}^{-1}$. The events selected had to satisfy a trigger requiring at least one loose photon candidate with $E_{T}>20 \mathrm{GeV}$, and had to contain at least one reconstructed primary vertex consistent with the average beam spot position and with at least three associated tracks. The trigger and vertex requirements are $\approx 99 \%$ efficient for signal MC events. The presence of multiple $p p$ collisions within the same bunch crossing, known as "pileup," can be analyzed by examining $N_{v t x}$, the number of reconstructed primary vertices in each event. In this data sample, the average value of $N_{v t x}$ was $\approx 2.1$. The MC signal samples included the simulation of pileup and were weighted to match the $N_{v t x}$ distribution observed in data.

Events were retained if they had at least two photon candidates, each with $E_{T}>25 \mathrm{GeV}$. In addition, a photon isolation cut was applied, wherein the $E_{T}$ in a radius of 0.2 in the $\eta-\phi$ space around the center of the cluster, excluding the cells belonging to the cluster in a region corresponding to $5 \times 7$ cells in $\eta \times \phi$ in the second layer of the EM calorimeter, had to be less than 35 GeV . This requirement had a signal efficiency greater than $95 \%$ but rejected some of the background from multijet events. An event in which each of the two photon candidates satisfied the loose photon cuts was considered a $\gamma \gamma$ candidate event. An independent "misidentified jet" control sample, enriched in events with jets misidentified as photons, was defined as those events where at least one of the photon candidates did not pass the loose photon identification. After all cuts, the $\gamma \gamma$ and misidentified jet samples totaled 520 and 7323 events, respectively. Figure 1 shows the $E_{T}$ spectrum of the leading photon for the $\gamma \gamma$ candidates and for UED $1 / R=700 \mathrm{GeV}$ MC events; the UED spectrum extends to much higher $E_{T}$ values.

The background was evaluated entirely using data. Noncollision backgrounds, such as cosmic rays and beam-halo events, are reduced to a negligible level by the


FIG. 1. $E_{T}$ spectrum of the leading photon for the $\gamma \gamma$ candidate sample and for UED $1 / R=700 \mathrm{GeV}$ MC events (normalized to 100 times the leading order (LO) cross section).
selection cuts. The main background source, referred to hereafter as QCD background, arises from a mixture of SM processes including $\gamma \gamma$ production, and $\gamma+$ jet and multijet events with at least one jet misidentified as a photon. With the loose photon identification, it is expected that $\gamma+$ jet and multijet events dominate, with only a small $\gamma \gamma$ contribution. The misidentified jet sample provided a model of the $E_{T}^{\text {miss }}$ response for events with jets faking photons. The response for $\gamma \gamma$ events was modeled using the $E_{T}^{\text {miss }}$ spectrum measured in a high purity sample of $Z \rightarrow e e$ events, selected by a combination of kinematic cuts and electron identification requirements [14]. The $E_{T}^{\text {miss }}$ spectrum for $Z \rightarrow e e$ events, which is dominated by the calorimeter response to two genuine EM objects, was verified in MC simulations to model the $E_{T}^{\text {miss }}$ response in SM $\gamma \gamma$ processes, despite their kinematic differences. As shown in Fig. 2, $Z \rightarrow e e$ events typically have somewhat lower $E_{T}^{\text {miss }}$ values than events of the misidentified jet sample, as expected since the presence of jets faking photons should result in a broader $E_{T}^{\text {miss }}$ distribution. The spectrum for the $\gamma \gamma$ candidates, which for low $E_{T}^{\text {miss }}$ is dominated by the QCD background with an unknown mixture of events with zero, one, and two fake photons, lies between these two samples. The $E_{T}^{\text {miss }}$ spectrum of the total QCD background was modeled by a weighted sum of the spectra of the $Z \rightarrow e e$ and misidentified jet samples. The QCD background was normalized to have the same number of events as the $\gamma \gamma$ candidate sample in the region $E_{T}^{\text {miss }}<20 \mathrm{GeV}$, where any UED signal contribution can


FIG. 2 (color online). $\quad E_{T}^{\text {miss }}$ spectra for the $\gamma \gamma$ candidates, for the $Z \rightarrow e e$ and misidentified jet samples used to model the QCD background (each normalized to the number of $\gamma \gamma$ candidates with $\left.E_{T}^{\text {miss }}<20 \mathrm{GeV}\right)$, and for the $W(\rightarrow e \nu)+$ jets $/ \gamma$ background (normalized to its expected total of $\approx 0.4$ events). Variable sized bins are used, and the vertical error bars and shaded bands show the statistical errors.
be neglected. The relative contributions of the $Z \rightarrow e e$ and misidentified jet samples were determined by fitting the QCD background shape to the $E_{T}^{\text {miss }}$ spectrum of the $\gamma \gamma$ candidates in this same low $E_{T}^{\text {miss }}$ region. The fraction attributed to $\gamma \gamma$ production, as modeled with the $Z \rightarrow e e$ distribution, was determined to be $(36 \pm 22) \%$. The search result is not very sensitive to the exact composition of the QCD background, and the fit error was used to determine systematic uncertainties on the background prediction.

A small additional background results from $W \rightarrow e v$ events, which have genuine $E_{T}^{\text {miss }}$ and which can pass the selection if the electron is misidentified as a photon and the second photon is either a real photon in $W \gamma$ events or a jet faking a photon in $W+$ jets events. A high purity sample of inclusive $W \rightarrow e v$ events was selected by a combination of kinematic and electron identification cuts [14]. Requiring in addition a loose photon with $E_{T}^{\gamma}>25 \mathrm{GeV}$, a " $W+\gamma$ " sample of only 5 events was selected. Accounting for the probability for an electron to be misidentified as a loose photon, as determined using the $Z \rightarrow e e$ sample, the total background contribution due to $W \rightarrow e v$ events was then estimated to be only $\approx 0.4$ events. Since the number of $W \gamma$ events was too small to measure their $E_{T}^{\text {miss }}$ spectrum, a sample of $W+$ jets events was used instead, requiring a jet reconstructed with an anti- $k_{T}$ clustering algorithm [16] with radius parameter 0.4 and $E_{T}^{j}>25 \mathrm{GeV}$. The $W(\rightarrow e \nu)+$ jets $/ \gamma$ background contribution was then estimated by normalizing the $W+$ jets $E_{T}^{\text {miss }}$ spectrum to the expected total of $\approx 0.4$ events, as shown on Fig. 2.

Figure 3 shows the $E_{T}^{\text {miss }}$ spectrum of the $\gamma \gamma$ candidates, superimposed on the total background prediction, as well


FIG. 3 (color online). $E_{T}^{\text {miss }}$ spectrum for the $\gamma \gamma$ candidates, compared to the total SM background as estimated from data. Also shown are the expected UED signals for $1 / R=500 \mathrm{GeV}$ and 700 GeV . Variable sized bins are used, and the vertical error bars and shaded bands show the statistical errors.

TABLE I. The number of observed $\gamma \gamma$ candidates, as well as the SM backgrounds estimated from data and expected UED signal for $1 / R$ values of 500 and 700 GeV , given in various $E_{T}^{\text {miss }}$ ranges. The uncertainties are statistical only. The first row, for $E_{T}^{\text {miss }}<20 \mathrm{GeV}$, is the control region used to normalize the QCD background to the number of observed $\gamma \gamma$ candidates.

| $E_{T}^{\text {miss }}$ range | Data |  | Predicted background events |  | Expected UED signal events |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| $(\mathrm{GeV})$ | events | Total | QCD | $W(\rightarrow e \nu)+$ jets $/ \gamma$ | $1 / R=500 \mathrm{GeV}$ | $1 / R=700 \mathrm{GeV}$ |
| $0-20$ | 465 | $465.0 \pm 9.1$ | $465.0 \pm 9.1$ | - | $0.28 \pm 0.06$ | $0.02 \pm 0.01$ |
| $20-30$ | 45 | $40.5 \pm 2.2$ | $40.41 \pm 2.17$ | $0.11 \pm 0.07$ | $0.45 \pm 0.07$ | $0.03 \pm 0.01$ |
| $30-50$ | 9 | $10.3 \pm 1.3$ | $10.13 \pm 1.30$ | $0.16 \pm 0.10$ | $1.60 \pm 0.12$ | $0.08 \pm 0.01$ |
| $50-75$ | 1 | $0.93 \pm 0.23$ | $0.85 \pm 0.23$ | $0.08 \pm 0.05$ | $2.84 \pm 0.16$ | $0.14 \pm 0.01$ |
| $>75$ | 0 | $0.32 \pm 0.16$ | $0.28 \pm 0.15$ | $0.04 \pm 0.03$ | $40.45 \pm 0.62$ | $4.21 \pm 0.06$ |

as example UED signals. Table I summarizes the number of observed $\gamma \gamma$ candidates, as well as the expected backgrounds and example UED signal contributions, in several $E_{T}^{\text {miss }}$ ranges. The QCD background dominates, and falls steeply with rising $E_{T}^{\text {miss }}$, while the $W \rightarrow e v$ background is very small, and flatter as a function of $E_{T}^{\text {miss }}$. The UED signals would peak at large values of $E_{T}^{\text {miss }}$. There is good agreement between the data and predicted background over the entire $E_{T}^{\text {miss }}$ range, with no indication of an excess at high $E_{T}^{\mathrm{miss}}$ values.

The signal search region was chosen to be $E_{T}^{\text {miss }}>$ 75 GeV , before looking at the data, to obtain the best sensitivity to the UED signal. In the signal region, there are zero observed events, compared to an expectation of $0.32 \pm 0.16(\text { stat })_{-0.10}^{+0.37}($ syst $)$ background events. The systematic uncertainty was derived by studying variations of the background determination, including varying within its error the $\gamma \gamma$ fraction determined in the fit of the QCD background, varying the definition of the misidentified jet sample, and eliminating the photon isolation cut.

The UED signal efficiency, determined from MC simulations, increases smoothly from $\approx 43 \%$ for $1 / R=500 \mathrm{GeV}$ to $\approx 48 \%$ for $1 / R=700 \mathrm{GeV}$, with the lower efficiencies for smaller $1 / R$ due mostly to the $E_{T}^{\text {miss }}>75 \mathrm{GeV}$ definition of the signal region. The various relative systematic uncertainties on the extraction of the UED signal cross section are summarized in Table II, including the dominant $11 \%$ uncertainty on the integrated luminosity [17]. Uncertainties on the efficiency for reconstructing and identifying the $\gamma \gamma$ pair arise mainly due to

TABLE II. Relative systematic uncertainties on the expected UED signal yield. For more details, see the text.

| Source of uncertainty | Uncertainty |
| :--- | :---: |
| Integrated luminosity | $11 \%$ |
| Photon reconstruction and identification | $4 \%$ |
| Effect of pileup | $2 \%$ |
| $E_{T}^{\text {miss }}$ reconstruction and scale | $1 \%$ |
| Signal MC statistics | $1 \%$ |
| Total | $12 \%$ |

differences between MC simulations and data in the distributions of the photon identification variables, the need to extrapolate to the higher $E_{T}$ values (see Fig. 1) typical of the UED photons, the impact of the photon quality cuts, varying the scale of the photon $E_{T}$ cut, and uncertainties in the detailed material composition of the detector. Together these provide a systematic uncertainty of $4 \%$. The influence of pileup, evaluated by comparing MC samples with and without pileup, gives a systematic uncertainty of $2 \%$. Systematic effects on the $E_{T}^{\text {miss }}$ reconstruction [14], including pileup, varying the cluster energies within the current uncertainties, and varying the expected $E_{T}^{\text {miss }}$ resolution between the measured performance and MC expectations, combine to give a $1 \%$ uncertainty on the signal efficiency. Finally, the $1 \%$ statistical error on the signal efficiency as determined by MC simulations is treated as a systematic uncertainty on the result. Adding in quadrature, the total systematic uncertainty on the signal yield is $12 \%$.

Given the good agreement between the measured $E_{T}^{\text {miss }}$ spectrum and the expected background, a limit was set on $1 / R$ in the specific UED model considered here. A Bayesian approach was used to calculate a limit based on the number of observed and expected events with $E_{T}^{\mathrm{miss}}>$ 75 GeV . A Poisson distribution was used as the likelihood function for the expected number of signal events, and a flat prior was used for the signal cross section. Log-normal priors were used for the various sources of uncertainty, which were treated as nuisance parameters. It was verified that the result is not very sensitive to the detailed form of the assumed priors. Figure 4 depicts the resulting 95\%C.L. upper limit within the context of the UED model considered, together with the LO UED cross section as a function of $1 / R$. The LO cross section was used since higher order corrections have not been calculated for the UED model. An uncertainty on the signal cross section due to parton distribution functions (PDF's) was determined by comparing the predictions using MRST2007 [18] PDF's with those from the full set of error PDF's of CTEQ6.6 [19]. The resultant uncertainty, namely $\pm 8 \%$ essentially independent of $1 / R$, is shown by the width of the theory curve band. The observed $95 \%$ C.L. exclusion region is $1 / R<$ 729 GeV . The result depends weakly on the systematic


FIG. 4 (color online). 95\%C.L. upper limits on the UED production cross section, and the LO theory cross section prediction, as a function of $1 / R$. The shaded band shows the PDF uncertainty.
uncertainties, and would only increase to 732 GeV if they were neglected. Changing the $E_{T}^{\text {miss }}$ cut to 60 or 90 GeV would change the limit by only a few GeV . A cross-check using a higher purity $\gamma \gamma$ sample, achieved by requiring that both photons pass tighter identification cuts that reject more of the background from jets, produced a consistent result.

In conclusion, a search for $\gamma \gamma$ events with large $E_{T}^{\text {miss }}$, conducted using a $3.1 \mathrm{pb}^{-1}$ sample of $7 \mathrm{TeV} p p$ collisions recorded with the ATLAS detector at the LHC, found no evidence of an excess above the SM prediction. The results were used to set limits on a specific model with one UED and gravity-induced LKP decays, excluding at the $95 \% \mathrm{C}$.L. values of $1 / R<729 \mathrm{GeV}$, and significantly surpassing the only existing experimental limit [7] on this model.

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# Measurement of Dijet Azimuthal Decorrelations in $p p$ Collisions at $\sqrt{s}=7 \mathrm{TeV}$ 

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#### Abstract

Azimuthal decorrelations between the two central jets with the largest transverse momenta are sensitive to the dynamics of events with multiple jets. We present a measurement of the normalized differential cross section based on the full data set ( $\int \mathcal{L} d t=36 \mathrm{pb}^{-1}$ ) acquired by the ATLAS detector during the $2010 \sqrt{s}=7 \mathrm{TeV}$ proton-proton run of the LHC. The measured distributions include jets with transverse momenta up to 1.3 TeV , probing perturbative QCD in a high-energy regime.


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The production of events containing high transversemomentum $\left(p_{T}\right)$ jets is a key signature of quantum chromodynamic ( QCD ) interactions between partons in $p p$ collisions at large center-of-mass energies $(\sqrt{s})$. The Large Hadron Collider (LHC) opens a window into the dynamics of interactions with high- $p_{T}$ jets in a new energy regime of $\sqrt{s}=7 \mathrm{TeV}$. QCD predicts the decorrelation in the azimuthal angle between the two most energetic jets, $\Delta \phi$, as a function of the number of partons produced. Events with only two high $-p_{T}$ jets have small azimuthal decorrelations, $\Delta \phi \sim \pi$, while $\Delta \phi \ll \pi$ is evidence of events with several high- $p_{T}$ jets. QCD also describes the evolution of the shape of the $\Delta \phi$ distribution, which narrows with increasing leading jet $p_{T}$. Distributions in $\Delta \phi$ therefore test perturbative QCD (pQCD) calculations for multiple jet production without requiring the measurement of additional jets. Furthermore, a detailed understanding of events with large azimuthal decorrelations is important to searches for new physical phenomena with dijet signatures, such as supersymmetric extensions to the standard model [1].

In this Letter, we present a measurement of dijet azimuthal decorrelations with jet $p_{T}$ up to 1.3 TeV as measured by the ATLAS detector, beyond the reach of previous colliders. The differential cross section $(1 / \sigma)(d \sigma / d \Delta \phi)$ is based upon an integrated luminosity $\int \mathcal{L} d t=$ ( $36 \pm 4$ ) $\mathrm{pb}^{-1}$ [2]. The $\Delta \phi$ distribution is normalized by the inclusive dijet cross section $\sigma$, integrated over the same phase space. This construction minimizes experimental and theoretical uncertainties. Previous measurements of $\Delta \phi$ from the D0 [3] and CMS [4] Collaborations are extended here to higher jet $p_{T}$ values.
Jets are reconstructed using the anti- $k_{t}$ algorithm [5] (implemented with FASTJET [6]) with radius $R=0.6$, and the jet four-momenta are constructed from a sum over its constituents, treating each as an $(E, \vec{p})$ four-vector with

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zero mass. The anti- $k_{t}$ algorithm is well motivated since it is infrared safe to all orders, produces geometrically welldefined conelike jets, and is used for PQCD calculations (from partons), event generators (from stable particles), and the detector (from energy clusters [7]). The azimuthal decorrelation $\Delta \phi$ is defined as the absolute value of the difference in azimuthal angle between the jet with the highest $p_{T}$ in each event, $p_{T}^{\max }$, and the jet with the second-highest $p_{T}$ in the event. There are nine analysis regions in $p_{T}^{\text {max }}$, where the lowest region is bounded by $p_{T}^{\max }>110 \mathrm{GeV}$ and the highest region requires $p_{T}^{\max }>$ 800 GeV [7]. Only jets with $p_{T}>100 \mathrm{GeV}$ and $|y|<2.8$, where $y$ is the jet rapidity [8], are considered. The two leading jets that define $\Delta \phi$ are required to satisfy $|y|<0.8$, restricting the measurement to a central $y$ region where the momentum fractions ( $x$ ) of the interacting partons are roughly equal and the experimental acceptance for multijet production is increased. In this region where $0.02 \leqslant x \lesssim$ 0.14 , the parton distribution function (PDF) uncertainties are typically $\pm 3 \%$ (at fixed factorization scale) [9]. The cross sections, measured over the range $\pi / 2 \leq \Delta \phi \leq \pi$ and normalized independently for each analysis region, are compared with expectations from a pQCD calculation [10] that is next-to-leading order (NLO) in three-parton production. The perturbative prediction for the cross section is $\mathcal{O}\left(\alpha_{s}^{4}\right)$, where $\alpha_{s}$ is the strong coupling constant.

The angular decorrelation is sensitive to multijet configurations such as those produced by event generators like SHERPA [11], which matches higher-order tree-level pQCD diagrams with a dipole parton-shower model [12]. Samples for $2 \rightarrow 2-6$ jet production are combined using an improved parton matching scheme [13]. Event generators such as PYTHIA [14] and HERWIG [15] use $2 \rightarrow 2$ leading order pQCD matrix elements matched with phenomenological parton-cascade models to simulate higher-order QCD effects. Such models have been successful at reproducing other QCD processes measured by the ATLAS Collaboration [7,16].

The ATLAS detector $[17,18]$ consists of an inner tracking system surrounded by a thin superconducting solenoid providing a 2 T magnetic field, electromagnetic and hadronic calorimeters, and a muon spectrometer based on
large superconducting toroids. Jet measurements depend most heavily on the calorimeters. The electromagnetic calorimeter is a lead liquid-argon (LAr) detector with an accordion geometry. Hadron calorimetry is based on two different detector technologies, with scintillator tiles or LAr as the active medium, and with either steel, copper, or tungsten as the absorber material. The pseudorapidity $(\eta)$ [8] and $\phi$ segmentations of the calorimeters are sufficiently fine to ensure that angular resolution uncertainties are negligible compared to other sources of systematic uncertainty.

A hardware-based calorimeter jet trigger identified events of interest; the decision was further refined in software $[17,18]$. Events with at least one jet that satisfied a minimum transverse energy $\left(E_{T}\right)$ requirement were recorded for further analysis. The events in each $p_{T}^{\max }$ range are selected by a single trigger with a given $E_{T}$ threshold, and the lower end of the range is chosen above the jet $p_{T}$ at which that trigger is $\approx 100 \%$ efficient. Three sets of triggered events with different integrated luminosity are considered: $2.3 \mathrm{pb}^{-1}$ for $110<p_{T}^{\max } \leq 160 \mathrm{GeV}, 9.6 \mathrm{pb}^{-1}$ for $160<p_{T}^{\max } \leq 260 \mathrm{GeV}$, and $36 \mathrm{pb}^{-1}$ for $p_{T}^{\max }>$ 260 GeV [2]. Events are also required to have a reconstructed primary vertex within 15 cm in $z$ of the center of the detector; each vertex had $\geq 5$ associated tracks. The inputs to the anti- $k_{t}$ jet algorithm are clusters of calorimeter cells seeded by cells with energy that is significantly above the measured noise [7]. Jets reconstructed in the detector, whether in data or the GEANT4-based simulation [19,20], are corrected for the effects of hadronic shower response and detector-material distributions using a $p_{T^{-}}$and $\eta$-dependent calibration [7] based on the detector simulation and validated with extensive test beam [18] and collision data [21] studies. Jets likely to have arisen from detector noise or cosmic rays are rejected [22].

The resulting $\Delta \phi$ distribution is shown in Fig. 1 for jets with $p_{T}>100 \mathrm{GeV}$. There are 146788 events in the data sample, 85 of which have at least five jets with $p_{T}>$ 100 GeV . Also shown is the PYTHIA sample with MRST 2007 LO* PDF [23] and ATLAS MC09 underlying event tune [24], processed through the full detector simulation and normalized to the number of events in the data sample. Two- and three-jet production primarily populates the region $2 \pi / 3<\Delta \phi<\pi$ while smaller values of $\Delta \phi$ require additional activity such as soft radiation or more jets in an event. Figure 1 illustrates that the decorrelation increases when a third high- $p_{T}$ jet is also required. Events with additional high- $p_{T}$ jets widen the overall distribution.

The measured differential $\Delta \phi$ distributions in data are corrected in a single step with a bin-by-bin unfolding method [7] to compensate for trigger and detector inefficiencies and the effects of finite experimental resolutions. These correction factors, evaluated using the PYTHIA sample, lie within $\pm 9 \%$ of unity. The leading sources of


FIG. 1 (color online). The $\Delta \phi$ distribution for $\geq 2, \geq 3, \geq 4$, and $\geq 5$ jets with $p_{T}>100 \mathrm{GeV}$. Overlaid on the calibrated but otherwise uncorrected data (points) are results from PYTHIA processed through the detector simulation (lines). All uncertainties are statistical only.
systematic uncertainty on the normalized cross section are the jet energy scale calibration ( $2 \%-17 \%$ ) [7], the bin-bybin unfolding method ( $1 \%-19 \%$ ), and the jet energy and position resolutions $(0.5 \%-5 \%)$. The ranges in parentheses represent the magnitude of the uncertainties near $\pi$ and $\pi / 2$, respectively, and correspond to the analysis region with the smallest statistical uncertainty $\left(160<p_{T}^{\max } \leq\right.$ 210 GeV ). Multiple $p p$ interactions in the same beam crossing that can increase the measured jet energy are included in the evaluation of the jet energy scale uncertainties $(<0.8 \%$ on the cross section for all analysis regions).

The normalized differential cross section is shown for each of the nine $p_{T}^{\max }$ analysis regions as a function of $\Delta \phi$ in Fig. 2. As $p_{T}^{\max }$ increases, and the probability for the emission of a hard third jet is reduced, the fraction of events near $\pi$ becomes larger. Overlaid on the data are the results from a NLO pQCD $\left[\mathcal{O}\left(\alpha_{s}^{4}\right)\right]$ calculation, NLOJET + + [10] with FASTNLO [25] and using the MSTW 2008 PDF [9]. The factorization and renormalization scales are set to $p_{T}^{\max }$ and are varied independently up and down by a factor of 2 to determine the scale uncertainties. The scale uncertainties are larger between $\pi / 2<$ $\Delta \phi<2 \pi / 3$ where the pQCD calculation is effectively leading order in four-parton production. The PDF uncertainties are treated as the envelope of the $68 \%$ C.L. uncertainties from MSTW 2008 [9], NNPDF 2.0 [26], and CTEQ 10 [27], and are combined with the uncertainties resulting from an $\alpha_{s}$ variation of $\pm 0.004$; the $\alpha_{s}$ contributions dominate. The calculation is corrected for nonperturbative effects due to hadronization and the underlying event [28]; the correction is smaller than $3 \%$. The fixedorder calculation fails near $\Delta \phi \rightarrow \pi$ where soft processes dominate and contributions from logarithmic terms are enhanced. Figure 3 displays the ratio of the cross section


FIG. 2 (color online). The differential cross section $(1 / \sigma) \times$ $(d \sigma / d \Delta \phi)$ binned in nine $p_{T}^{\max }$ regions. Overlaid on the data (points) are results from the NLO pQCD calculation. The error bars on the data points indicate the statistical (inner error bar) and systematic uncertainties added in quadrature in this and subsequent figures. The theory uncertainties are indicated by the hatched regions. Different bins in $p_{T}^{\max }$ are scaled by multiplicative factors of 10 for display purposes. The region near the divergence at $\Delta \phi \rightarrow \pi$ is excluded from the calculation.
with respect to the NLO calculation. In most regions, the theory is consistent with the data. However, the prediction in the range $110<p_{T}^{\max }<160 \mathrm{GeV}$ is relatively low in the central region of $\Delta \phi$ where the scale uncertainties are small.

The data are also compared with predictions [29] from sherpa, pythia, and herwig in Fig. 4. The leadinglogarithmic approximations used in these event generators' parton-shower models effectively regularize the divergence at $\Delta \phi \rightarrow \pi$; all three provide a good description of the data in this region. In the region $\pi / 2<\Delta \phi<5 \pi / 6$, where multijet contributions are significant, this observable distinguishes between the three generators. SHERPA, which explicitly includes higher-order tree-level diagrams, performs well in most $\Delta \phi$ and $p_{T}^{\max }$ regions. Having phenomenological parameters that have been adjusted to previous ATLAS measurements, PYTHIA [28] and HERWIG [24] also describe the data.

In summary, we present a measurement of dijet azimuthal decorrelations in events produced in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$. The normalized differential cross sections


FIG. 3 (color online). Ratio of the differential cross section $(1 / \sigma)(d \sigma / d \Delta \phi)$ measured in data with respect to expectations from NLO pQCD (points). The theory uncertainties are indicated by the hatched regions. The region near the divergence at $\Delta \phi \rightarrow \pi$ is excluded from the comparison.
are based on the full data set ( $\int \mathcal{L} d t=36 \mathrm{pb}^{-1}$ ) collected by the ATLAS Collaboration during the 2010 run of the LHC. Expectations from NLO pQCD $\left[\mathcal{O}\left(\alpha_{s}^{4}\right)\right]$ and those of


FIG. 4 (color online). Ratio of the differential cross section $(1 / \sigma)(d \sigma / d \Delta \phi)$ measured in data with respect to the result from SHERPA (points). The shaded region indicates the SHERPA statistical uncertainty. Predictions from PYTHIA and HERWIG, also in ratio to SHERPA, are displayed as lines.
several event generators successfully describe the general characteristics of our measurements, including the increasing slope of the $\Delta \phi$ distribution with $p_{T}^{\max }$ and the shape near $\Delta \phi \sim \pi / 2$ where events with multiple jets make a considerable contribution. Our data, which include jets with $p_{T}$ values that significantly exceed earlier measurements, explore QCD in a new kinematic region.

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Piccinini, ${ }^{19 a, 19 b}$ A. Pickford, ${ }^{53}$ S. M. Piec, ${ }^{41}$ R. Piegaia, ${ }^{26}$ J. E. Pilcher, ${ }^{30}$ A. D. Pilkington, ${ }^{82}$ J. Pina, ${ }^{124 a, c}$ M. Pinamonti, ${ }^{164 a, 164 \mathrm{c}}$ A. Pinder, ${ }^{118}$ J. L. Pinfold, ${ }^{2}$ J. Ping, ${ }^{32 \mathrm{c}}$ B. Pinto, ${ }^{124 \mathrm{a}, \mathrm{c}}$ O. Pirotte, ${ }^{29}$ C. Pizio, ${ }^{89 \mathrm{a}, 89 \mathrm{~b}}$ R. Placakyte, ${ }^{41}$ M. Plamondon, ${ }^{169}$ W. G. Plano,,${ }^{82}$ M.-A. Pleier, ${ }^{24}$ A. V. Pleskach, ${ }^{128}$ A. Poblaguev,,${ }^{24}$ S. Poddar, ${ }^{58 a}$ F. Podlyski, ${ }^{33}$ L. Poggioli, ${ }^{115}$ T. Poghosyan,,${ }^{20}$ M. Pohl, ${ }^{49}$ F. Polci, ${ }^{55}$ G. Polesello, ${ }^{119 \mathrm{a}}$ A. Policicchio, ${ }^{138}$ A. Polini, ${ }^{19 a}$ J. Poll, ${ }^{75}$ V. Polychronakos, ${ }^{24}$ D. M. Pomarede,,${ }^{136}$ D. Pomeroy, ${ }^{22}$ K. Pommès, ${ }^{29}$ L. Pontecorvo, ${ }^{132 a}$ B. G. Pope,,${ }^{88}$ G. A. 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# Search for Dilepton Resonances in $p p$ Collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS Detector 

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#### Abstract

This Letter reports on a search for narrow high-mass resonances decaying into dilepton final states. The data were recorded by the ATLAS experiment in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ at the Large Hadron Collider and correspond to a total integrated luminosity of $1.08(1.21) \mathrm{fb}^{-1}$ in the $e^{+} e^{-}\left(\mu^{+} \mu^{-}\right)$channel. No statistically significant excess above the standard model expectation is observed and upper limits are set at the $95 \%$ C.L. on the cross section times branching fraction of $Z^{\prime}$ resonances and Randall-Sundrum gravitons decaying into dileptons as a function of the resonance mass. A lower mass limit of 1.83 TeV on the sequential standard model $Z^{\prime}$ boson is set. A Randall-Sundrum graviton with coupling $k / \bar{M}_{\mathrm{P} 1}=0.1$ is excluded at 95\% C.L. for masses below 1.63 TeV .


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This Letter describes a search for narrow high-mass resonances decaying into $e^{+} e^{-}$or $\mu^{+} \mu^{-}$pairs using $7 \mathrm{TeV} p p$ collision data recorded with the ATLAS detector [1]. Such resonances, which are predicted by several extensions of the standard model (SM), include new heavy spin-1 neutral gauge bosons such as $Z^{\prime}[2-4]$ and $Z^{*}[5]$, technimesons [6-8], as well as spin-2 Randall-Sundrum (RS) gravitons $G^{*}$ [9].

The benchmark models considered for the $Z^{\prime}$ are the sequential standard model (SSM) [2], with the same couplings to fermions as the $Z$ boson, and the $E_{6}$ grand unified symmetry group [4], broken into $S U(5)$ and two additional $U(1)$ groups, leading to new neutral gauge fields $\psi$ and $\chi$. The particles associated with the additional fields can mix in a linear combination to form the $Z^{\prime}$ candidate: $Z^{\prime}\left(\theta_{E_{6}}\right)=$ $Z_{\psi}^{\prime} \cos \theta_{E_{6}}+Z_{\chi}^{\prime} \sin \theta_{E_{6}}$, where $\theta_{E_{6}}$ is the mixing angle between the two gauge bosons. The pattern of spontaneous symmetry breaking and the value of $\theta_{E_{6}}$ determine the $Z^{\prime}$ couplings to fermions; six well-motivated choices of $\theta_{E_{6}}$ $[2,4]$ lead to the specific $Z^{\prime}$ states named $Z_{\psi}^{\prime}, Z_{N}^{\prime}, Z_{\eta}^{\prime}, Z_{I}^{\prime}$, $Z_{S}^{\prime}$, and $Z_{\chi}^{\prime}$.

Other models predict additional spatial dimensions as a possible explanation for the gap between the electroweak symmetry breaking scale and the gravitational energy scale. The RS model [9] predicts excited Kaluza-Klein modes of the graviton, which appear as spin-2 resonances. These modes have a narrow intrinsic width when $k / \bar{M}_{\mathrm{PI}}<0.1$, where $k$ is the spacetime curvature in the extra dimension and $\bar{M}_{\mathrm{Pl}}=M_{\mathrm{Pl}} / \sqrt{8 \pi}$ is the reduced Planck scale.

Previous searches have set direct and indirect constraints on the mass of the $G^{*}$ and $Z^{\prime}$ resonances [10,11]. The

[^35]Tevatron $[12,13]$ experiments exclude a $Z_{\text {SSM }}^{\prime}$ with a mass lower than 1.071 TeV [13]. Recent measurements from the LHC experiments, based on $\approx 40 \mathrm{pb}^{-1}$ of data recorded in 2010, exclude a $Z_{\text {SSM }}^{\prime}$ with a mass lower than 1.042 TeV (ATLAS) [14] and 1.140 TeV (CMS) [15]. Indirect constraints from LEP [16-19] extend these limits to 1.787 TeV [11]. Constraints on the mass of the RS graviton have been set by the CMS [15], CDF [20], and D0 [21] Collaborations, excluding RS gravitons with mass below 1.079 TeV for $k / \bar{M}_{\mathrm{Pl}}=0.1[15]$.

The ATLAS detector consists of inner tracking devices surrounded by a 2 T superconducting solenoid, electromagnetic and hadronic calorimeters, and a muon spectrometer with a toroidal magnetic field. Charged particles in the pseudorapidity range $|\eta|<2.5$ [22] are reconstructed with the inner detector, which consists of silicon pixel, silicon strip, and transition radiation detectors. The superconducting solenoid is surrounded by a hermetic calorimeter that covers $|\eta|<4.9$. For $|\eta|<2.5$, the electromagnetic calorimeter is finely segmented and plays an important role in electron identification. Outside the calorimeter, air-core toroids provide the magnetic field for the muon spectrometer. Three sets of precision drift tubes and cathode strip chambers provide an accurate measurement of the muon track curvature in the region $|\eta|<2.7$. Resistive-plate and thin-gap chambers provide muon triggering capability up to $|\eta|<2.4$.

The data sample used in this analysis, recorded during the first half of 2011, corresponds to a total integrated luminosity of $1.08(1.21) \mathrm{fb}^{-1}$ in the $e^{+} e^{-}\left(\mu^{+} \mu^{-}\right)$channel. Events are required to pass single electron (muon) triggers with a transverse energy $E_{T}$ (transverse momentum $p_{T}$ ) threshold above $20(22) \mathrm{GeV}$. Collision candidates are selected by requiring a primary vertex with at least three associated charged particle tracks with $p_{T}>0.4 \mathrm{GeV}$.

In the $e^{+} e^{-}$channel, two electron candidates are required with transverse energy $E_{T}>25 \mathrm{GeV}$ and $|\eta|<2.47$; the transition region $1.37 \leq|\eta| \leq 1.52$
between the barrel and the end cap calorimeters is excluded. Electron candidates are formed from clusters of cells reconstructed in the electromagnetic calorimeter associated with a charged particle track in the inner detector. Criteria on the transverse shower shape, the longitudinal leakage into the hadronic calorimeter, and the association with an inner detector track are applied to the cluster to define a so-called medium electron [23,24]. The electron energy is obtained from the calorimeter measurement and its direction from the associated track. A hit in the first active pixel layer is required to suppress background from photon conversions. To further suppress background from QCD jet production, the higher $E_{T}$ electron is required to be isolated by demanding that $\Sigma E_{T}(\Delta R<0.2)<$ 7 GeV , where $\Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}$ and $\Sigma E_{T}(\Delta R<0.2)$ is the sum of the transverse energies around the electron direction. The core of the electron energy deposition is excluded and the sum is corrected for transverse shower leakage and pileup from additional $p p$ collisions. The two electron candidates are not required to have opposite charge to minimize the impact of possible charge misidentification. For these selection criteria, the total signal acceptance for a $Z^{\prime} \rightarrow e^{+} e^{-}\left(G^{*} \rightarrow e^{+} e^{-}\right)$of mass 1.5 TeV is $65 \%$ ( $69 \%$ ), and is approximately independent of mass above 600 GeV . These numbers include the acceptance of all selection cuts and efficiencies and reflect the lepton angular distributions due to spin.

In the $\mu^{+} \mu^{-}$channel, two muon candidates of opposite charge are required, each satisfying $p_{T}>25 \mathrm{GeV}$. Muon tracks are reconstructed independently in both the inner detector and muon spectrometer, and their momenta are determined from a combined fit to these two measurements. To optimize the momentum resolution, each muon candidate is required to pass quality cuts in the inner detector and to have at least three hits in each of the inner, middle, and outer layers of the muon system. Muons with hits in both the barrel and the end cap regions are discarded because of residual misalignment between these two parts of the muon spectrometer. The effects of misalignments and intrinsic position resolution are included in the simulation. The $p_{T}$ resolution at 1 TeV ranges from $15 \%$ (central) to $44 \%$ (for $|\eta|>2$ ).

To suppress background from cosmic rays, the muon tracks are required to have a transverse impact parameter $\left|d_{0}\right|<0.2 \mathrm{~mm}$, a distance along the beam line to the primary vertex below 1 mm , and the $z$ position of the primary vertex $|z(\mathrm{PV})|<200 \mathrm{~mm}$. To reduce background from QCD jets, each muon is required to be isolated such that $\Sigma p_{T}(\Delta R<0.3) / p_{T}(\mu)<0.05$, where only tracks with $p_{T}>1 \mathrm{GeV}$ enter the sum. The total signal acceptance is $40 \%(44 \%)$ for a $Z^{\prime} \rightarrow \mu^{+} \mu^{-}\left(G^{*} \rightarrow \mu^{+} \mu^{-}\right)$of mass 1.5 TeV . The lower acceptance compared to the electron channel is due to the stringent requirements on the muon selection criteria to improve $p_{T}$ resolution.

For both channels, the dominant and irreducible background is due to the $Z / \gamma^{*}$ (Drell-Yan) process, characterized by the same final state as the signal. Small contributions from $t \bar{t}$ and diboson ( $W W, W Z$, and $Z Z$ ) production are also present in both channels. Semileptonic decays of $b$ and $c$ quarks in the $\mu^{+} \mu^{-}$ sample and a mixture of photon conversions, semileptonic heavy quark decays, and hadrons faking electrons in the $e^{+} e^{-}$sample are backgrounds that are referred to below as QCD background. Jets accompanying $W$ bosons ( $W+$ jets) may similarly produce lepton candidates.

The expected signal and backgrounds, with the exception of the QCD component, are evaluated with simulated samples and rescaled using the most precise available cross section predictions. The $Z^{\prime}, G^{*}$ signal, and $Z / \gamma^{*}$ processes are generated with PYTHIA 6.421 [25] using MRST2007 LO* [26] parton distribution functions (PDFs). Interference between the $Z / \gamma^{*}$ processes and the heavy resonances is small and therefore neglected. The diboson processes are generated with HERWIG 6.510 [27] using MRST2007 LO* PDFs. The $W+$ jets background is generated with ALPGEN [28] using CTEQ6L1 [29] PDFs and the $t \bar{t}$ background with MC@NLO 3.41 [30] using CTEQ66 [31]


FIG. 1 (color online). Dielectron (top) and dimuon (bottom) invariant mass ( $m_{\ell \ell}$ ) distribution after final selection, compared to the stacked sum of all expected backgrounds, with three example $Z_{\text {SSM }}^{\prime}$ signals overlaid. The bin width is constant in $\log m_{\ell \ell}$.

TABLE I. Expected and observed number of events in the dielectron (top) and dimuon (bottom) channels. The first bin is used to normalize the total background to the data. The errors quoted include both statistical and systematic uncertainties, except the error on the total background in the normalization region which is given by the square root of the number of observed events. The systematic uncertainties are correlated across bins and are discussed in the text.

| $m_{e^{+} e^{-}}[\mathrm{GeV}]$ | $70-110$ | $110-200$ | $200-400$ | $400-800$ | $800-3000$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Drell-Yan | $258482 \pm 410$ | $5449 \pm 180$ | $613 \pm 26$ | $53.8 \pm 3.1$ | $2.8 \pm 0.1$ |
| $t \bar{t}$ | $218 \pm 36$ | $253 \pm 10$ | $82 \pm 3$ | $5.4 \pm 0.3$ | $0.1 \pm 0.0$ |
| Diboson | $368 \pm 19$ | $85 \pm 5$ | $29 \pm 2$ | $3.1 \pm 0.5$ | $0.3 \pm 0.1$ |
| $W+$ jets | $150 \pm 100$ | $150 \pm 26$ | $43 \pm 10$ | $4.6 \pm 1.8$ | $0.2 \pm 0.4$ |
| QCD | $332 \pm 59$ | $191 \pm 75$ | $36 \pm 29$ | $1.8 \pm 1.4$ | $<0.05$ |
| Total | $259550 \pm 510$ | $6128 \pm 200$ | $803 \pm 40$ | $68.8 \pm 3.9$ | $3.4 \pm 0.4$ |
| Data | 259550 | 6117 | 808 | 65 | 3 |
| $m_{\mu^{+} \mu^{-}[G e V]}$ | $70-110$ | $110-200$ | $200-400$ | $400-800$ | $800-3000$ |
| Drell-Yan | $236319 \pm 320$ | $5171 \pm 150$ | $483 \pm 22$ | $40.3 \pm 2.5$ | $2.0 \pm 0.3$ |
| $t \bar{t}$ | $193 \pm 21$ | $193 \pm 20$ | $63 \pm 6$ | $4.2 \pm 0.4$ | $0.1 \pm 0.0$ |
| Diboson | $307 \pm 16$ | $69 \pm 5$ | $25 \pm 2$ | $1.7 \pm 0.5$ | $<0.05$ |
| $W+$ jets | $1 \pm 1$ | $1 \pm 1$ | $<0.5$ | $<0.05$ | $<0.05$ |
| QCD | $1 \pm 1$ | $<0.5$ | $<0.5$ | $46.1 \pm 2.6$ | $<0.05$ |
| Total | $236821 \pm 487$ | 5434150 | $571 \pm 23$ | 51 | $2.1 \pm 0.3$ |
| Data | 236821 |  | 557 | 5 |  |

PDFs. For both, JIMMY 4.31 [32] is used to describe multiple parton interactions and HERWIG to describe the remaining underlying event and parton showers. Final-state photon radiation is handled with PHOTOS [33]. The samples are processed through a full ATLAS detector simulation [34] based on GEANT4 [35].

The $Z / \gamma^{*}$ cross section is calculated at next-to-next-toleading order (NNLO) using PHOZPR [36] with MSTW2008 PDFs [37]. The ratio of this cross section to the leadingorder cross section is used to determine a mass-dependent QCD $K$ factor which is applied to the results of the leadingorder simulations. The same QCD $K$ factor is applied to the $Z^{\prime}$ signal. No QCD $K$ factor is available for $G^{*}$ production at $7 \mathrm{TeV}[38,39]$. Higher-order weak corrections (beyond the photon radiation included in the simulation) are calculated using HORACE $[40,41]$, yielding a weak $K$ factor due to virtual heavy gauge boson loops. The weak $K$ factor is only applied to the Drell-Yan background. The diboson cross sections are calculated to next-to-leading order (NLO) using MCFM [42] with an uncertainty of $5 \%$. The $W+$ jets cross section is rescaled to the inclusive NNLO
calculation of FEWZ [43], resulting in 30\% uncertainty when at least one parton with $E_{T}>20 \mathrm{GeV}$ accompanies the $W$ boson. The $t \bar{t}$ cross section is predicted at approximate NNLO, with $10 \%$ uncertainty [44,45].

The QCD background in the $e^{+} e^{-}$sample is estimated with data using "reversed electron identification" and "isolation fit" techniques [14], and a third method that uses fake rates measured from inclusive jet samples. In the reversed electron identification technique, data with both electron candidates failing some identification criteria (chosen not to affect kinematic distributions) are used to determine the QCD background distribution versus $m_{e e}$. This method is used for the central estimate and the others which bracket it, to assign a systematic uncertainty. The QCD background in the $\mu^{+} \mu^{-}$sample is evaluated from data using the muon isolation variable $\Sigma p_{T}(\Delta R<0.3) / p_{T}$ [14]. The QCD and $W+$ jets backgrounds are small (negligible) for the electron (muon) channel. Backgrounds from cosmic rays are negligible.

The observed invariant mass distributions are compared to the SM expectation. For this purpose, the Drell-Yan, $t \bar{t}$,

TABLE II. Summary of the dominant systematic uncertainties on the expected signal and background yields at $m_{\ell^{+} \ell^{-}}=1.5 \mathrm{TeV}$ for the $Z^{\prime}\left(G^{*}\right)$ analysis.

| Source | Dielectrons |  | Dimuons |  |
| :--- | :---: | :---: | :---: | :---: |
|  | Signal | Background | Signal | Background |
| Normalization | $5 \%$ | Not applicable | $5 \%$ | Not applicable |
| PDFs $/ \alpha_{S}$ | Not applicable | $10 \%$ | Not applicable | $10 \%$ |
| QCD $K$ factor | Not applicable | $3 \%$ | Not applicable | $3 \%$ |
| Weak $K$ factor | Not applicable | $4.5 \%$ | Not applicable | $4.5 \%$ |
| Trigger/reconstruction | Negligible | Negligible | $4.5 \%$ | $4.5 \%$ |
| Total | $5 \%$ | $11 \%$ | $7 \%$ | $12 \%$ |

diboson and $W+$ jets backgrounds from Monte Carlo simulation are scaled according to their respective cross sections and added to the QCD background. The simulated backgrounds are then rescaled so that the sum matches the observed number of data events in the $70-110 \mathrm{GeV}$ mass interval. The scaling factor is within $1 \%$ of unity. The advantage of this approach is that the uncertainty on the luminosity, and any mass independent uncertainties on efficiencies, cancel between the $Z^{\prime}\left(G^{*}\right)$ and the $Z$ boson.

Figure 1 presents the invariant mass ( $m_{\ell \ell}$ ) distribution for the dielectron (top) and dimuon (bottom) final states after final selection, while Table I shows the number of data events and the estimated backgrounds in bins of reconstructed $m_{\ell \ell}$. The dilepton invariant mass distributions are well described by the prediction from SM processes. Figure 1 also displays the expected $Z_{\text {SSM }}^{\prime}$ signal for three mass hypotheses.

The invariant mass distribution of the data is compared to the backgrounds and signal templates with pole masses in the $0.13-2.0 \mathrm{TeV}$ range $[14,46]$. A likelihood function is


FIG. 2 (color online). Expected and observed 95\% C.L. upper limits on $\sigma B$ as a function of mass for $Z^{\prime}$ (top) and $G^{*}$ (bottom) models. Both results show the combination of the electron and muon channels. The thickness of the $Z_{\text {SSM }}^{\prime}$ (top) and the $G^{*}$ for $k / \bar{M}_{\mathrm{Pl}}=0.1$ (bottom) theory curves illustrate the theoretical uncertainties.
defined as the product of the Poisson probabilities over all mass bins in the search region. The Poisson probability in each bin is evaluated for the observed number of data events given the background and signal template expectation. The total signal acceptance as a function of mass is propagated into the expectation.

The significance of a signal is summarized by a $p$ value, the probability of observing an excess at least as signal-like as the one observed in data, in the absence of signal. The outcome of the search is ranked using a likelihood ratio, which is scanned as a function of $Z^{\prime}$ cross section and $m_{Z^{\prime}}$ over the full considered mass range. The data are consistent with the SM hypothesis, with $p$ values of $54 \%$ and $24 \%$ for the $e^{+} e^{-}$and $\mu^{+} \mu^{-}$channels, respectively.

Given the absence of a signal, an upper limit on the signal cross section is determined at the $95 \%$ C.L. using a Bayesian approach [47] with a flat, positive prior on the signal cross section.

Mass-dependent systematic uncertainties are incorporated as nuisance parameters which are integrated out [47]. They include normalization to the $Z$ peak, PDF, QCD, and weak $K$ factors, as well as trigger, reconstruction, and identification efficiencies. These uncertainties are correlated across all bins in the search region and they are correlated between signal and background.

Since the total background is normalized to the data in the region of the $Z \rightarrow \ell^{+} \ell^{-}$mass peak, the residual systematic uncertainties are small at the $Z$ pole and grow at higher mass. The dominant uncertainties are theoretical. The overall uncertainty due to PDF and $\alpha_{S}$ variations is estimated to be $10 \%$ at 1.5 TeV using the MSTW 2008 eigenvector PDF sets and other PDF sets corresponding to variations of $\alpha_{S}$. The difference with respect to CTEQ is included as an additional 3\% uncertainty. The uncertainty on the QCD $K$ factor is $3 \%$, evaluated from variations of the renormalization and factorization scales by factors of two around the nominal values. A systematic uncertainty of $4.5 \%$ is attributed to electroweak corrections [14]. The uncertainty on the $Z / \gamma^{*}$ cross section is $5 \%$, which is applied as a systematic uncertainty on the normalization.

Experimental systematic effects due to resolution and inefficiencies at high mass were studied. In the electron channel, the calorimeter energy resolution is dominated at large $E_{T}$ by a constant term which is $1.2 \%$ in the barrel and $1.8 \%$ in the end caps, with negligible uncertainty. The uncertainty on the resolution in the muon channel is due to residual misalignments and intrinsic position uncertainties in the muon spectrometer that propagate to a change in

TABLE III. Observed (expected) 95\% C.L. mass lower limits in TeV on $Z_{\mathrm{SSM}}^{\prime}$ resonance and $G^{*}$ graviton (with $k / \bar{M}_{\mathrm{PI}}=0.1$ ).

| Model | $e^{+} e^{-}$ | $\mu^{+} \mu^{-}$ | $\ell^{+} \ell^{-}$ |
| :--- | :---: | :---: | :---: |
| $Z_{\mathrm{SSM}}^{\prime}$ | $1.70(1.70)$ | $1.61(1.61)$ | $1.83(1.83)$ |
| $G^{*}$ | $1.51(1.50)$ | $1.45(1.44)$ | $1.63(1.63)$ |

TABLE IV. $\quad 95 \%$ C.L. lower limits on the masses of $E_{6}$-motivated $Z^{\prime}$ bosons and RS gravitons $G^{*}$ for various values of the coupling $k / \bar{M}_{\mathrm{Pl}}$. Both lepton channels are combined.

|  | $E_{6} Z^{\prime}$ models |  |  |  |  |  | RS graviton |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Model/coupling | $Z_{\psi}^{\prime}$ | $Z_{N}^{\prime}$ | $Z_{\eta}^{\prime}$ | $Z_{I}^{\prime}$ | $Z_{S}^{\prime}$ | $Z_{\chi}^{\prime}$ | 0.01 | 0.03 | 0.05 | 0.1 |
| Mass limit [TeV] | 1.49 | 1.52 | 1.54 | 1.56 | 1.60 | 1.64 | 0.71 | 1.03 | 1.33 | 1.63 |

the observed width of the $Z^{\prime}\left(G^{*}\right)$ line shape. The simulation was adjusted to reproduce the data at high muon momentum. The residual uncertainty translates into an event yield uncertainty of less than $1.5 \%$. The combined uncertainty on the muon trigger and reconstruction efficiency is estimated to be $4.5 \%$ at 1.5 TeV . This uncertainty is dominated by a conservative estimate of the impact of large energy loss from muon bremsstrahlung in the calorimeter on the muon reconstruction performance in the muon spectrometer. In the electron channel, a systematic uncertainty of $1.5 \%$ at 1.5 TeV is estimated for a possible identification inefficiency caused by the isolation requirement.

The dominant systematic uncertainties are summarized in Table II. Uncertainties below 3\% are neglected, and no theory uncertainties are applied to the $Z^{\prime}$ or $G^{*}$ signal in the limit setting procedure described below.

The limit on the number of produced $Z^{\prime}\left(G^{*}\right)$ events is converted into a limit on cross section times branching fraction $\sigma B$ by scaling with the observed number of $Z$ boson events and the theoretical value of $\sigma B(Z \rightarrow l l)$. The expected exclusion limits are determined using simulated pseudoexperiments containing only standard model processes, by evaluating the $95 \%$ C.L. upper limits for each pseudoexperiment for each fixed value of $m_{Z^{\prime}}\left(m_{G^{*}}\right)$. The median of the distribution of limits represents the expected limit. The ensemble of limits is used to find the $68 \%$ and $95 \%$ envelopes of the expected limits as a function of $m_{Z^{\prime}}$ $\left(m_{G^{*}}\right)$. Figure 2 (top) shows the combined dielectron and dimuon $95 \%$ C.L. observed and expected exclusion limits on $\sigma B\left(Z^{\prime} \rightarrow l l\right)$. It also shows the theoretical cross section times branching fraction for the $Z_{\mathrm{SSM}}^{\prime}$ and for $E_{6}$-motivated $Z^{\prime}$ models with the lowest and highest $\sigma B$. Figure 2 (bottom) shows the corresponding limits on the RS graviton. Mass limits obtained for the $Z_{\text {SSM }}^{\prime}$ and $G^{*}$ (with $k / \bar{M}_{\mathrm{Pl}}=0.1$ ) are displayed in Table III. The combined mass limits on the $E_{6}$-motivated models and the $G^{*}$ with various couplings are given in Table IV.

In conclusion, the ATLAS detector has been used to search for narrow, heavy resonances in the dilepton invariant mass spectrum above the $Z$ boson pole. Proton-proton collision data with $1.08(1.21) \mathrm{fb}^{-1}$ in the $e^{+} e^{-}\left(\mu^{+} \mu^{-}\right)$ channel have been used. The observed invariant mass spectra are consistent with the SM expectations. Limits are set on the cross section times branching fraction $\sigma B$. The resulting mass limits are 1.83 TeV for the sequential standard model $Z^{\prime}$ boson, $1.49-1.64 \mathrm{TeV}$ for various $E_{6}$-motivated $Z^{\prime}$ bosons, and $0.71-1.63 \mathrm{TeV}$ for a

Randall-Sundrum graviton with couplings $\left(k / \bar{M}_{\mathrm{PI}}\right)$ in the range $0.01-0.1$. The $Z^{\prime}$ boson limits are the most stringent to date, including indirect limits set by LEP2.

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# Search for Magnetic Monopoles in $\sqrt{s}=7$ TeV $p p$ Collisions with the ATLAS Detector 

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#### Abstract

This Letter presents a search for magnetic monopoles with the ATLAS detector at the CERN Large Hadron Collider using an integrated luminosity of $2.0 \mathrm{fb}^{-1}$ of $p p$ collisions recorded at a center-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$. No event is found in the signal region, leading to an upper limit on the production cross section at $95 \%$ confidence level of $1.6 / \epsilon \mathrm{fb}$ for Dirac magnetic monopoles with the minimum unit magnetic charge and with mass between 200 GeV and 1500 GeV , where $\epsilon$ is the monopole reconstruction efficiency. The efficiency $\epsilon$ is high and uniform in the fiducial region given by pseudorapidity $|\eta|<1.37$ and transverse kinetic energy $600-700<E^{\mathrm{kin}} \sin \theta<1400 \mathrm{GeV}$. The minimum value of 700 GeV is for monopoles of mass 200 GeV , whereas the minimum value of 600 GeV is applicable for higher mass monopoles. Therefore, the upper limit on the production cross section at $95 \%$ confidence level is 2 fb in this fiducial region. Assuming the kinematic distributions from Drell-Yan pair production of spin- $1 / 2$ Dirac magnetic monopoles, the efficiency is in the range $1 \%-10 \%$, leading to an upper limit on the cross section at $95 \%$ confidence level that varies from 145 fb to 16 fb for monopoles with mass between 200 GeV and 1200 GeV . This limit is weaker than the fiducial limit because most of these monopoles lie outside the fiducial region.


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Magnetic monopoles have long been the subject of dedicated search efforts for three main reasons: their introduction into the theory of electromagnetism would restore the symmetry between electricity and magnetism in Maxwell's equations; their existence would explain the quantization of electric charge [1]; and they appear in many grand unified theories [2]. However, to date no experimental evidence of a magnetically charged object exists.

Recent searches for magnetic monopoles from astrophysical sources [3-9] are complemented by searches at colliders [10-14]. This Letter describes a search for magnetic monopoles in proton-proton collisions recorded at a center-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ using the ATLAS detector at the CERN Large Hadron Collider (LHC).

The Dirac quantization condition [1], given in Gaussian units, leads to a prediction for the minimum unit magnetic charge $g$,

$$
\begin{equation*}
\frac{g e}{\hbar c}=\frac{1}{2} \Rightarrow \frac{g}{e}=\frac{1}{2 \alpha_{e}} \approx 68.5, \tag{1}
\end{equation*}
$$

where $e$ is the unit electric charge and $\alpha_{e}$ is the fine structure constant. With the introduction of a magnetic monopole, the duality of Maxwell's equations implies a magnetic coupling [15]

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$$
\begin{equation*}
\alpha_{m}=\frac{(g \beta)^{2}}{\hbar c}=\frac{1}{4 \alpha_{e}} \beta^{2}, \tag{2}
\end{equation*}
$$

where $\beta=v / c$ is the monopole velocity. For relativistic monopoles, $\alpha_{m}$ is very large, precluding any perturbative calculation of monopole production processes. Therefore, the main result of this analysis is a fiducial cross-section limit for Dirac monopoles of magnetic charge $g$ derived without assuming a particular production mechanism. A cross-section limit assuming the kinematic distributions from Drell-Yan monopole pair production is also provided.

Monopoles are highly ionizing particles, interacting with matter like an ion of electric charge $68.5 e$, according to Eq. (1). The high stopping power of the monopole ionization [16] results in the production of a large number of $\delta$ rays. These energetic "knock-on" electrons emitted from the material carry away energy from the monopole trajectory and further ionize the medium. In the mass and energy regime of this study, the $\delta$ rays have kinetic energies ranging from 1 MeV to a maximum of $\sim 100 \mathrm{MeV}$. The secondary ionization by these $\delta$ rays represents a significant fraction of the ionization energy loss of the magnetic monopole [16]. The dominant energy loss mechanism for magnetic monopoles in the mass and energy range considered herein is ionization [16-18]. Furthermore, the monopole ionization is independent of the monopole speed $\beta$ to first order, in contrast to the ionization of electrically charged particles.

In the ATLAS detector [19,20], the monopole signature can be easily distinguished using the transition radiation tracker (TRT) in the inner detector and the liquid argon (LAr) sampling electromagnetic (EM) calorimeter.

The TRT is a straw-tube tracker that comprises a barrel ( $|\eta|<1.0$ ) with 4 mm diameter straws oriented parallel to the beam line, and two end caps $(0.8<|\eta|<2.0)$ with straws orientated radially. A minimum ionizing particle deposits $\sim 2 \mathrm{keV}$ of energy in a TRT straw. Energy deposits in a TRT straw greater than 200 eV (called "low-threshold hits'") are used for tracking, while those that exceed 6 keV (called "high-threshold hits") typically occur due to the transition radiation emitted by highly relativistic electrons when they penetrate the radiator layers between the straws. As a result, an electron of energy 5 GeV or above has a $20 \%$ probability of producing a high-threshold hit in any straw it traverses. The high-threshold hits can also indicate the presence of a highly ionizing particle. A 2 T superconducting solenoid magnet surrounds the inner detector. The LAr barrel EM calorimeter lies outside the solenoid in the $|\eta|<1.5$ region. It is divided into three shower-depth layers and comprises accordion-shaped electrodes and lead absorbers. The cell granularity in the second layer is $\Delta \eta \times \Delta \phi=0.025 \times 0.025$. The characteristic signature of magnetic monopoles in ATLAS is a large localized energy deposit in the LAr EM calorimeter (EM cluster) in conjunction with a region of high ionization density in the TRT. A search for particles with large electric charge, which yield a similar signature, was performed previously [21] and production cross-section limits for such particles were set [22].
The trajectory of an electrically neutral magnetic monopole in the inner detector is straight in the $r-\phi$ plane and curved in $r-z$. The behavior of magnetic monopoles in the ATLAS detector is described by a GEANT4 [23] simulation [24], which includes the equations of motion, the ionization, the $\delta$-ray production and a modified Birks' law [25] to model recombination effects in LAr due to highly ionizing particles [26]. Equation 5.5 in Ref. [16] gives the $\delta$-ray production cross section and Eq. 5.7 describes the derivation of the magnetic monopole ionization; both equations are implemented in GEANT4.

Simulated Monte Carlo (MC) single-monopole samples are used to determine the efficiency as a function of the transverse kinetic energy $E_{\mathrm{T}}^{\text {kin }}=E^{\text {kin }} \sin \theta$ and pseudorapidity $\eta$ for various monopole masses. For the Drell-Yan process, it is assumed that spin- $1 / 2$ magnetic monopoles are produced in pairs from the initial $p p$ state via quarkantiquark annihilation into a virtual photon. MADGRAPH [27] is used to model this process by assuming leadingorder Drell-Yan heavy lepton pair production but making the replacement $e \rightarrow g \beta$ to reflect the magnetic coupling in Eq. (2). In the absence of a consistent theory describing the coupling of the monopole to the $Z$ boson, such a coupling is set to zero in the madgraph model. In the Drell-Yan samples, the CTEQ6L1 [28] parton distribution functions are used and PYTHIA version 6.425 [29] is used for the hadronization and the underlying event. Only DrellYan monopoles with transverse momentum $p_{\mathrm{T}}>200 \mathrm{GeV}$
are processed by the simulation since lower $p_{\mathrm{T}}$ monopoles fail to reach the calorimeter. For all the simulated samples, both the monopoles and the antimonopoles are assumed to be stable and all final-state particles are processed by the simulation of the ATLAS detector. Additional $p p$ collisions in each event are simulated according to the distribution of $p p$ interactions per bunch crossing in the selected data period.

A simple algorithm is used to preselect events with monopole candidates for further study. Monopoles with $E_{\mathrm{T}}^{\mathrm{kin}}$ above approximately 500 GeV traverse the inner detector and penetrate to the LAr calorimeter, depositing most of their energy there. Only one third of the deposited energy is recorded due to the recombination effects in LAr [26]. Lacking a dedicated monopole trigger, only events collected with a single-electron trigger with transverse energy threshold $E_{\mathrm{T}}>60 \mathrm{GeV}$ are considered. This trigger requires a track in the inner detector within $|\Delta \eta|<0.01$ and $|\Delta \phi|<0.02$ of the LAr energy deposit. Monopoles that fulfill the 60 GeV energy requirement travel fast enough to satisfy the tracking and timing requirements of the trigger. Very high-energy monopoles (i.e., those with $E_{\mathrm{T}}^{\text {kin }} \gtrsim 1400-1900 \mathrm{GeV}$, where the value of 1400 GeV is for monopoles of mass 1500 GeV and the value of 1900 GeV is for monopoles of mass 200 GeV ) exit the EM calorimeter and are rejected by a veto on hadronic energy that is intrinsic to the single-electron trigger. This trigger was operational during the first six months of 2011 data-taking and recorded an integrated luminosity of $2.0 \mathrm{fb}^{-1}$, defining the data set used for this search.

The reconstructed EM cluster is then required to have $E_{\mathrm{T}}>65 \mathrm{GeV}$ and $|\eta|<1.37$. The trigger efficiency is independent of $E_{T}$ for $E_{\mathrm{T}}>65 \mathrm{GeV}$, motivating the former requirement. The $\eta$ requirement ensures that the EM cluster is in the barrel region of the LAr calorimeter, where the two-dimensional spatial resolution is uniform. If two or more EM clusters in an event satisfy these criteria, only the cluster with the highest energy is considered as a monopole candidate.

In the barrel region, the monopole typically traverses 35 TRT straws and its high ionization ensures that most of these register high-threshold hits. Furthermore, as each $\delta$ ray produced by the monopole ionization deposits $\sim 2 \mathrm{keV}$ in a straw, the combined energy deposited by multiple $\delta$ rays crossing a single TRT straw gives rise to additional high-threshold hits. The large number of $\delta$ rays bend in the 2 T magnetic field in the $r$ - $\phi$ plane; therefore, the monopole trajectory appears as a $\sim 1$-cm-wide swath of highthreshold TRT hits. The fraction of TRT hits that exceed the high threshold in the vicinity of the path of an ionizing particle is therefore a powerful discriminator between the monopole signal and the background. The $\phi$ position of the EM cluster is used to define a road of width $\Delta \phi= \pm 0.05 \mathrm{rad}$ from the beam line to the cluster. At least 20 high-threshold TRT hits must be present in the
road. In addition, at least $20 \%$ of the TRT hits in the road must be high-threshold hits.

After the preselection, a more refined TRT hit counting algorithm is used to distinguish the signal from the backgrounds. A histogram with a bin width of 0.8 mrad is filled with the $\phi$ distribution of the high-threshold hits in the previously defined road. The location of the highest bin is used to calculate the center of a new road. In the TRT barrel, a rectangular road of $\pm 4 \mathrm{~mm}$ in the $r-\phi$ plane is used and the hits are counted. In the TRT end cap, a wedgeshaped road of width $\Delta \phi= \pm 0.006 \mathrm{rad}$ is used. These roads are wide enough to encompass two neighboring straws, taking into account the monopole trajectory and the associated $\delta$ rays, but sufficiently narrow to ensure that the fraction of hits that exceed the high threshold, $f_{\mathrm{HT}}$, is insensitive to the presence of neighboring tracks. In the barrel region, the number of hits in the road is required to be greater than 54 . An $\eta$-dependent requirement on the number of hits in the road is applied in the end cap and barrel-end-cap transition region to account for the TRT geometry.

Energy loss by bremsstrahlung and $e^{+} e^{-}$pair production is negligible for magnetic monopoles in the mass and energy range considered herein. Therefore, magnetic monopoles give rise to a narrow ionization energy deposit in the LAr calorimeter, the size of which provides another powerful discriminator of the monopole signal from backgrounds such as electrons and photons, which induce an EM shower via bremsstrahlung and $e^{+} e^{-}$pair production. The variable used is $\sigma_{\mathrm{R}}$, the energy-weighted two-dimensional $\eta-\phi$ cluster dispersion in the second layer of the EM calorimeter, which has the highest two-dimensional spatial resolution. The dispersion $\sigma_{\mathrm{R}}$ is calculated from the energies deposited in a $3 \times 7$ array of cells centered around the most energetic cell of the EM cluster: $\sigma_{\mathrm{R}}=\sqrt{\sigma_{\phi}^{2}+\sigma_{\eta}^{2}}$, where $\sigma_{\phi}^{2}=\Sigma\left(E_{i} \delta \phi_{i}^{2}\right) / \Sigma E_{i}-\left[\Sigma\left(E_{i} \delta \phi_{i}\right) / \Sigma E_{i}\right]^{2}, \delta \phi_{i}$ is the deviation in $\phi$ between cell $i$ and the most energetic cell, and $E_{i}$ is the energy of cell $i ; \sigma_{\eta}^{2}$ is defined similarly.

The high-threshold TRT hit fraction, $f_{\mathrm{HT}}$, and the cluster dispersion, $\sigma_{\mathrm{R}}$, are thus chosen as the distinguishing variables between the signal and background, and are shown in Fig. 1. The main physics background sources are highenergy electrons, photons, and jets, which exhibit no correlation between these variables in simulated processes. The background and monopole MC samples are used to define an approximate signal region. Then ( $\sigma_{\mathrm{R}}, f_{\mathrm{HT}}$ ) parameter pairs are generated by randomly sampling the onedimensional $\sigma_{\mathrm{R}}$ and $f_{\mathrm{HT}}$ distributions for data outside this approximate signal region. The borders of the signal region are tuned for maximal significance of observation of three signal events by replacing the background MC events with these parameter pairs. The final signal region $A$ is defined by $\sigma_{\mathrm{R}} \leq 0.017$ and $f_{\mathrm{HT}}>0.7$.

The efficiencies, which include trigger, reconstruction, and selection effects, in the two-dimensional $E_{\mathrm{T}}^{\text {kin }}$ versus $\eta$


FIG. 1 (color online). High-threshold TRT hit fraction, $f_{\mathrm{HT}}$, versus EM cluster dispersion, $\sigma_{\mathrm{R}}$. The circles represent 1000 simulated single monopoles with mass 800 GeV . The crosses represent ATLAS data. The regions marked $A, B, C$, and $D$ are discussed in the text.
plane are obtained from the simulated single-monopole samples. A fiducial region for each monopole mass is defined by the $E_{\mathrm{T}}^{\mathrm{kin}}$ range in which the efficiency is 0.80 or higher in the $|\eta|<1.37$ region. Figure 2 shows the efficiency versus $E_{T}^{\text {kin }}$, averaged over $|\eta|<1.37$. For monopoles with a mass of 200 GeV , the minimum transverse kinetic energy $\left(E_{\mathrm{T}}^{\mathrm{kin}}\right)_{\min }$ where the efficiency rises above 0.80 is 700 GeV . For monopoles with a mass between 500 GeV and $1500 \mathrm{GeV},\left(E_{\mathrm{T}}^{\mathrm{kin}}\right)_{\min }$ is 600 GeV . Monopoles with lower $E_{\mathrm{T}}^{\mathrm{kin}}$ fail to penetrate to the EM calorimeter and therefore do not satisfy the trigger requirements. Monopoles with very high $E_{\mathrm{T}}^{\text {kin }}$ exit the EM calorimeter and are rejected by the hadronic veto of the electron trigger. A common upper value of $E_{\mathrm{T}}^{\mathrm{kin}}=$ 1400 GeV is used for the fiducial region of all monopole masses. As the minimum efficiency is 0.80 in the fiducial


FIG. 2 (color online). Efficiency versus $E_{T}^{\text {kin }}$, averaged over $|\eta|<1.37$, for single monopoles of mass 200 GeV and mass 1500 GeV .
region, a common value of 0.80 is used in the determination of the upper cross-section limit.

The efficiencies can be under- or overestimated for several reasons. These effects are described below and the relative systematic uncertainties for each effect are given. (1) Cross talk in the second EM layer in the $\phi$ direction is not modeled in the simulation. The energy is reweighted assuming $1.8 \%$ cross talk [30] and the cluster dispersion, $\sigma_{\mathrm{R}}$, recomputed. The efficiency is reduced and the resulting relative shift of $-1.7 \%$ for single monopoles is taken as a one-sided uncertainty. (2) The simulation underestimates the TRT occupancy in the data by up to $20 \%$; therefore, the number of low-threshold hits (those unlikely to come from the monopole or related $\delta$ rays) is increased by $20 \%$. The resulting relative uncertainty is $-1.3 \%$. (3) The modification to Birks' law is varied between its upper and lower systematic uncertainties [26], yielding a relative uncertainty of $+1.8 \%$ and $+1.5 \%$, respectively. (4) The production of $\delta$ rays is varied by $3 \%$ [16] and the resulting uncertainty is negligible.
(5) The GEant4 "range cut" [23] controls the minimum kinetic energy threshold below which $\delta$ rays are not propagated explicitly. This parameter is reduced from $50 \mu \mathrm{~m}$ to $25 \mu \mathrm{~m}$ in the TRT simulation. The resulting relative uncertainty is $+0.14 \%$. (6) The material in the inner detector, in the barrel cryostat and in between the cryostat and the first layer of the EM calorimeter is increased by $5 \%, 10 \%$, and $5 \%$, respectively, in the simulation [31]. The resulting $-0.74 \%$ relative uncertainty is taken as symmetric. Including an uncertainty of $\sim 1.7 \%$ to account for the limited number of MC events, the total upper and lower relative uncertainties on the efficiency for single monopoles are $+2.6 \%$ and $-2.8 \%$, respectively.

The efficiencies to reconstruct at least one of the monopoles in the pairs produced with Drell-Yan kinematic distributions are given in Table I for each mass. Only masses up to 1200 GeV are considered, taking into account the phase space limitations for pair production. The total relative uncertainties, which reflect the same systematic variations described above, are also given. The efficiencies and their associated systematic uncertainties reflect large losses due to acceptance, since many Drell-Yan monopoles have insufficient energy to reach the calorimeter.

The background in the signal region is predicted directly from the data. The two-dimensional plane in Fig. 1 is divided into quadrants, one of which is dominated by

TABLE I. Efficiencies and their relative uncertainties in percent for Drell-Yan pair-produced monopoles of various masses.

| Mass $(\mathrm{GeV})$ | 200 | 500 | 800 | 1000 | 1200 |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Efficiency | 0.011 | 0.048 | 0.081 | 0.095 | 0.095 |
| Relative uncertainty |  |  |  |  |  |
| Upper (\%) | +32 | +24 | +22 | +23 | +20 |
| Lower (\%) | -36 | -23 | -22 | -25 | -25 |

signal (region $A$ ), and three others that are occupied mainly by background (regions $B, C$, and $D$ ). The ratio of background events in signal region $A$ to events in background region $B$ is expected to be the same as the ratio of background events in regions $C$ to $D$. This assumption is incorporated into a maximum likelihood fit to determine the estimated numbers of signal and background events in signal region $A$. The inputs to the fit include the observed event yields in quadrants $A$ through $D$, which are $0,5,16$, and 7001, respectively, the efficiencies and associated systematic uncertainties that have already been discussed, and the integrated luminosity and its $3.7 \%$ uncertainty [32]. For each monopole mass, the rate of appearance of signal events in quadrants $B$ and $C$, as predicted by the simulation, is also taken into account. According to the simulation, no signal event appears in quadrant $D$ for any monopole mass. The fit predicts $0.011 \pm 0.007$ background events in the signal region.

Using the results of the maximum likelihood fit, the upper limits on the production cross sections at $95 \%$ confidence level are calculated using the profile likelihood ratio as a test statistic [33]. The results are extracted using the $C L_{s}$ method [34]. The cross-section limits can be expressed as a function of the efficiency, $\boldsymbol{\epsilon}$, which is shown in Fig. 2 for single monopoles and given in Table I for Drell-Yan pair-produced monopoles. The upper limit on the production cross section at $95 \%$ confidence level is found to be $1.6 / \epsilon$ fb for Dirac magnetic monopoles with the minimum unit magnetic charge and with mass between 200 GeV and 1500 GeV . Assuming the kinematic distributions from Drell-Yan pair production of spin-1/2 Dirac magnetic monopoles, this translates to an upper limit on the cross section at $95 \%$ confidence level that varies from 145 fb to 16 fb for monopoles with mass between 200 GeV and 1200 GeV , as shown in Fig. 3. Since the number of expected background events is very small and no event is


FIG. 3 (color online). Upper limits on the monopole production cross sections at $95 \%$ confidence level. The solid line is the limit for single monopoles in the fiducial region and the dashed line is the limit assuming the kinematic distributions from Drell-Yan (DY) monopole pair production.
observed in the signal region, only the observed limits are shown. To compare with previous experiments that have provided lower mass limits on spin-1/2 Dirac magnetic monopoles by assuming Drell-Yan pair production, such an approach would yield a lower mass limit of 862 GeV in the present search [35].

The monopole reconstruction efficiency is high and uniform in the fiducial region given by pseudorapidity $|\eta|<1.37$ and transverse kinetic energy $\left(E_{\mathrm{T}}^{\mathrm{kin}}\right)_{\text {min }}<$ $E^{\text {kin }} \sin \theta<1400 \mathrm{GeV}$, where $\left(E_{\mathrm{T}}^{\mathrm{kin}}\right)_{\min }$ is 600 GeV for monopoles with a mass between 500 GeV and 1500 GeV . For monopoles with a mass of $200 \mathrm{GeV},\left(E_{\mathrm{T}}^{\mathrm{kin}}\right)_{\min }=$ 700 GeV . Therefore, the upper limit on the production cross section at $95 \%$ confidence level is 2 fb , as shown in Fig. 3, for Dirac magnetic monopoles with the minimum unit magnetic charge and with mass between 200 GeV and 1500 GeV in this fiducial region. The fluctuations of the observed limit in the fiducial region originate from variations of the nuisance parameters used in the profile likelihood ratio.

These results extend the upper limits on the production cross section for monopoles in this mass region established by preceding experiments. This is the first direct collider search that yields cross-section constraints on magnetic monopoles with masses greater than 900 GeV .

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# ASIC developments for high speed serial data transmission in particle physics experiments 

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## A R T I C L E IN F O

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#### Abstract

We report R\&D results on two integrated circuit designs: a 5 Gbps $16: 1$ serializer and a 5 GHz LC phase-locked-loop (PLL). The prototypes were fabricated with a commercial thin-film silicon-on-sapphire $0.25 \mu \mathrm{~m}$ CMOS technology. Both the serializer and the PLL have been evaluated to meet design goals and tested against operation conditions in the environment of a particle physics detector front-end for the proposed HL-LHC upgrade.


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## 1. Introduction

Serial data transmission over optical fibers is used in particle physics experiments. The transmitting data rate over a single fiber channel increased from a few megabits per second (Mbps) to 1.6 gigabits per second (Gbps. Example: the optical link that reads out the Liquid Argon Calorimeter [1], or LAr, in the ATLAS experiment at CERN). The operation environments require high system reliability due to lack of frequent access for maintenance or repair. In some cases the radiation in a particle physics detector front-end also puts special requirements on the electronics and optics that operate inside the detector volume [2]. In the upgrade program for the High Luminosity Large Hadron Collider (HL-LHC) at CERN, R\&D projects are carried out to meet the challenges of higher radiation tolerance and system reliability, and much higher data bandwidth with low power dissipation, compared with the optical link systems now operating in experiments on the LHC. This is because with the increase of radiation in the detector front-end, it is advantageous to simplify the front-end readout electronics by moving all level- 1 triggering circuits to the back-end data acquisition (DAQ) system where frequent access is possible and there is no or very little radiation in the operation environment. The price to pay in the data-streaming mode frontend electronics is on the data transmission bandwidth. Taking the ATLAS LAr optical link as an example, the data throughput will increase from 1.6 Gbps per front-end board (FEB) to over 100 Gbps per FEB. To meet this challenge, and to address the needs in many new detectors' readout R\&D, especially those designs to operate in radiation environment, we have been

[^39]working on designs of Application Specific Integrated Circuits (ASICs) for the transmitting side of an optical link. The final goal of data throughput in our R\&D program is 10 Gbps per fiber. As a step towards that goal, we prototyped a $16: 1$ serializer designed to operate at 5 Gbps , and an LC based phase-locked-loop (PLL) that runs up to 5 GHz . Both designs are based on a commercial thin-film silicon-on-sapphire (SOS) $0.25 \mu \mathrm{~m}$ CMOS technology. The design and measurement results of the serializer are reported in Section 2, while those for the LC-PLL in Section 3. In the conclusion we point out our roadmap to the final goal of ASICs and the link system of 10 Gbps per fiber, or an aggregated bandwidth of 120 Gbps per FEB.

## 2. Design and measurement results of the $\mathbf{5} \mathbf{G b p s}$ serializer ASIC

A functional block diagram of serial data transmission over fiber optics is shown in Fig. 1. The interface block prepares the upstream parallel data for serial transmission hence works at a clock rate that is close to the parallel data clock which is much lower (by about $8 \times$ in this case) than the serial data rate. The serializer and the optical interface blocks have circuits that work at the highest clock frequency of the system. For example, for a 5 Gbps serial data rate and circuits using both edges of the clock, one needs a 2.5 GHz PLL. The optical interface consists of a (current) laser driver (LD) circuit and a laser. The LD is the same as a CML line driver with matching modulation current and impedance of the laser in use. Because of these, we decided to first prototype a 16:1 serializer with a CML output to gain experience with this SOS technology. To increase the chances of success, this design is also based on a ring oscillator PLL as its clock unit, learned from a successful previous ASIC serializer, the

GOL chip, developed for particle physics [3]. This PLL limits the serial speed to be 5 Gbps . To probe the speed of the technology, we also implemented a standalone LC based PLL. The design and testing of this serializer are described in the following subsections while the LC-PLL is described in Section 3.

### 2.1. The design of the ASIC

The design of the serializer follows an inverted tree structure with a cascade of many $2: 1$ multiplexing units, as shown in Fig. 2. The advantage of this serializing structure are twofold: one, the multiplexers operate at lower speeds except the last stage which runs at the final serial data rate, offering the possibility of "trading power for speed" only in the last multiplexer which is specially designed; two, the power-of-2 structure simplifies the design of the clock unit, which in this particular design is shared with the PLL divider chain. A divide-by-two divider immediately after the VCO (voltage controlled oscillator) in the PLL also helps to maximize the clock speed. The disadvantage of this structure is a serializing ratio of the power of 2 , requiring a possible data reformatting at the interface stage in front of the serializer. Since in most applications such an interface ASIC will be needed to perform many functions such as data framing, scrambling, redundancy switch, and communication for control and monitoring, adding data bus reformatting to the interface to cope with a particular application is manageable. The high-speed clock is synthesized based a ring-oscillator-PLL, also illustrated in Fig. 2. The PLL can be selected to latch to either the rising or the falling


Fig. 1. Block diagram of a fiber optics based serial link system.
edge of the reference clock (the parallel input data clock), ensuring correctly clocking in the input data. A selection of PLL low pass filter bandwidth is implemented to cope with different input clock quality. A static D-Flip-Flop is used to improve the serializer's immunity to single event upset caused by ionizing particles. To achieve the needed speed with these static DFF, its internal clock and clock-bar are carefully adjusted to ensure the shortest D-to-Q time.

### 2.2. The evaluation of the prototype

Testing of the prototype chip was carried out by wire-bonding it to a PCB. Special caution was exercised for a few very fast signals both in the PCB design with impedance-matched traces and in placing the chip for wire-bonding with the shortest connecting wires. In general electric signal reflection is minimized by implementing impedance match for all differential signal traces. For CMOS signal traces, resistors are placed in series to reduce sharp rising (falling) edge. Shown in Fig. 3(a) is the eye diagram measurement with an eye mask. A bathtub curve is also traced with a Bit-Error-Rate-Tester (Anritsu MP1763C/1764C) and is shown in Fig. 3(b). From both measurements one can extract an eye opening of 0.69 UI (Unit Interval). Signal rise/fall time, amplitude of a $100 \Omega$ differential load, timing jitter in the serial bit stream, together with different jitter components are listed in Table 1. The measured power consumption of this ASIC is 463 mW , corresponding to $93 \mathrm{~mW} / \mathrm{Gbps}$. This measured power consumption in room temperature agrees with simulation within $5 \%$.

### 2.3. The next step in serializer design

Making use of the fact that in most particle physics detector front-end electronics, all readout channels are based on one system clock, we decided to design an array serializer, with two serializing units sharing one LC-PLL. The choice of this architecture is a balance of power saving and high-speed clock distribution. A block diagram of this design is shown in Fig. 4. The designed serial data rate is 8 Gbps , as shown in the post-layout simulation of the output eye diagram. The simulated power consumption of this ASIC is 1200 mW , or $75 \mathrm{~mW} / \mathrm{Gbps}$. This design reaches the highest achievable serial data rate with the particular process we choose in this SOS technology, with all the constraints we have, in particular the radiation tolerance requirement.


Fig. 2. Block diagram design of the 16:15 Gbps serializer.
a

b


Fig. 3. (a) Eye diagram. (b) Bathtub scan of a 5 Gbps signal with $2^{7}-1$ PRBS input.

Table 1
Measurement results of the 5 Gbps serializer ASIC. Errors listed in the table are statistic only.

| Parameters (unit) | Value |
| :--- | :---: |
| Amplitude (V) | $1.16 \pm 0.03$ |
| Rise time (ps) | $52.0 \pm 0.9$ |
| Fall time (ps) | $51.9 \pm 1.0$ |
| Total jitter @ BER $10^{-12}(\mathrm{ps})$ | $61.6 \pm 6.9$ |
| Random jitter (ps) | $2.6 \pm 0.6$ |
| Total deterministic jitter (DJ) (ps) | $33.4 \pm 6.7$ |
| DJ: Periodic (ps) | $3.0 \pm 2.3$ |
| DJ: Inter-symbol interference | $3.0 \pm 2.3$ |
| (ps) |  |
| DJ: Duty cycle (ps) | $15.2 \pm 3.8$ |

## 3. Design and measurement results of the $\mathbf{5 G H z}$ LC-PLL

The chosen SOS technology offers high Q inductors. To take advantage of this, we designed an LC based PLL in the same prototype submission of the serializer, so one finds reusing many of the functional blocks from that serializer design. The challenge in the design is the varactor, the voltage controlled capacitor, of which the manufacturer does not provide a model for simulation. Due to schedule and budget constraints, we put a test bank of varactors together with the LC-PLL design in the same submission. Reported below are the results of the varactors and the LC-PLL.

### 3.1. The varactor results

Several varactors based on the RN and IN transistors are implemented in the prototype chip and are tested using LCR meters from Agilent (Model 4263B) and from Stanford Research System (SR720). The tests were carried out with frequencies from 100 Hz to 100 kHz , provided by the LCR meters. The tests were also carried out at room temperature and at liquid nitrogen temperature. Shown in Fig. 5 are the capacitance changes as a function of the bias voltage with the RN and IN transistor based varactors. Also shown are the simulation results. We use the RN transistors in our design. There is a systematic shift between simulated value and measured capacitance. Since the manufacturer does not provide a reliable simulation model for the varactors, we decide to take the measured value in our future designs.


Fig. 4. Block diagram of a 2-lane array serializer design.

### 3.2. The design of the ASIC and the measurement results

Block diagram of the LC-PLL is shown in Fig. 6. We reuse the phase-frequency-detector circuit (PFD), the charge-pump circuit (CP) and the low-pass-filter (LPF) from the ring-oscillator PLL inside the serializer. The first stage divider is a new design and works at 5 GHz . In order to test the design, and for lack of a 5 GHz output driver (we now know this is not possible with the chosen technology), we reuse the 2.5 GHz CML Driver for the signal output. We split the signal after the first divider stage, connecting one branch to the CML Driver. This is illustrated in Fig. 6. Based on


Fig. 5. Simulated and measured capacitance of RN (left) and IN (right) type of varactors.


Fig. 6. Block diagram of the LC-PLL with the CML output for testing purpose.

Table 2
Measurement results of the 5 GHz LC-PLL ASIC. Errors listed in the table are statistic only.

| Parameters (unit) | Value |
| :--- | :--- |
| Tuning frequency range (GHz) | $4.63 \pm 0.12$ to $4.98 \pm 0.02$ |
| Power consumption (mW) | $111 \pm 8$ |
| Output amplitude, pk-pk (V) | $1.23 \pm 0.09$ |
| Rise time (ps) | $44.9 \pm 2.4$ |
| Fall time (ps) | $44.4 \pm 2.2$ |
| Random jitter (ps) | $1.3 \pm 0.3$ |
| Deterministic jitter (ps) | $7.5 \pm 1.1$ |

simulated varactor tuning range, we thought that we should have a tuning range from 3.8 GHz to 5.0 GHz of the PLL. A mistake in the first divider design limited this range to be from 4.6 GHz to 5.0 GHz. This problem has been traced to a design mistake in the first stage divider and will be corrected in future designs. Listed in Table 2 are the results of this LC-PLL. The power consumption does not include those from the CML Driver and the LVDS receiver.

## 4. Conclusion

With one MPW run, we have 5 designs. Reported here are the results of a serializer, a LC-PLL and a testing block of varactors.

Built on these experiences, we are now designing LOCs2, and LOCld for the optical interface. Simulation results indicate that both LOCs2 and LOCld should work at 8 Gbps and this is really what this technology can offer. We will need either change the system design to work with the speed of 8 Gbps per fiber, or move to a newer SOS technology to reach higher speeds. The low speed (below 1 GHz ) and mostly digital circuits interface function block to complete the link transmitting side will be investigated at a later stage.

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# Limits on the production of the standard model Higgs boson in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

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#### Abstract

A search for the Standard Model Higgs boson at the Large Hadron Collider (LHC) running at a centre-ofmass energy of 7 TeV is reported, based on a total integrated luminosity of up to $40 \mathrm{pb}^{-1}$ collected by the ATLAS detector in 2010. Several Higgs boson decay channels: $H \rightarrow \gamma \gamma$, $H \rightarrow Z^{(*)} \rightarrow \ell \ell \ell \ell, H \rightarrow Z Z \rightarrow \ell \ell \nu \nu, H \rightarrow Z Z \rightarrow \ell \ell q q$, $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ and $H \rightarrow W W \rightarrow \ell \nu q q(\ell$ is e, $\mu)$ are combined in a mass range from 110 GeV to 600 GeV . The highest sensitivity is achieved in the mass range between 160 GeV and 170 GeV , where the expected $95 \%$ CL exclusion sensitivity is at Higgs boson production cross sections 2.3 times the Standard Model prediction. Upper limits on the cross section for its production are determined. Models with a fourth generation of heavy leptons and quarks with Standard Model-like couplings to the Higgs boson are also investigated and are excluded at $95 \%$ CL for a Higgs boson mass in the range from 140 GeV to 185 GeV .


## 1 Introduction

The search for the Standard Model Higgs boson [1-3] is one of the key aims of the Large Hadron Collider (LHC) at CERN. Prior to the LHC, the best direct information is a lower limit of 114.4 GeV , set using the combined results of the four LEP experiments [4], and an excluded band of 158 GeV to 173 GeV from the combined Tevatron experiments [5, 6]. First results from the ATLAS experiment are available in various Standard Model Higgs boson search channels [7-11]. There are also results from the CMS collaboration [12] in the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu^{1}$ channel which have a sensitivity similar to the equivalent search reported

[^40][^41]here. These results are based on proton-proton collision data collected in 2010 at a centre-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$. This paper combines the results from the different Higgs boson searches to obtain the overall sensitivity to a Standard Model Higgs boson with the 2010 ATLAS dataset.

All analyses use the most detailed calculations available for the cross sections, as discussed in Sect. 3. The searches in individual Higgs boson decay channels $H \rightarrow \gamma \gamma, H \rightarrow$ $W W^{(*)}$ and $H \rightarrow Z Z^{(*)}$ are outlined in Sects. 4, 5, and 6, respectively. The statistical interpretation uses the profilelikelihood ratio [13] as test-statistic. Thirty-one Higgs boson masses, in steps of 10 GeV from 110 GeV to 200 GeV (plus 115 GeV in addition) and 20 GeV from 200 GeV to 600 GeV , are tested. Exclusion limits are obtained using the power constrained $\mathrm{CL}_{\mathrm{s} b}$ limit [14], as discussed in Sect. 7. To allow for comparisons with the exclusion limits obtained by other experiments, the results are also determined using the $\mathrm{CL}_{s}$ method [15]. The limits are presented in terms of $\sigma / \sigma_{S M}$, the multiple of the expected Standard Model cross section at the Higgs boson mass considered. Results are also presented in terms of the corresponding ratio where the cross section in the denominator includes the effects of a fourth generation of heavy leptons and quarks with Standard Model-like couplings to the Higgs boson. Section 8 describes the treatment of the major sources of systematic uncertainty in the combined likelihood. The limits for individual channels and the combined results are detailed in Sect. 9 and the conclusions are drawn in Sect. 10.

## 2 The ATLAS detector

The ATLAS experiment [16] is a multipurpose particle physics apparatus with forward-backward symmetric cylindrical geometry covering $|\eta|<2.5$ for tracks and $\mid \eta<4.5$ for jets. ${ }^{2}$ The inner tracking detector (ID) consists of a sili-

[^42]con pixel detector, a silicon microstrip detector (SCT), and a transition radiation tracker (TRT). The ID is surrounded by a thin superconducting solenoid providing a 2 T magnetic field, and by high-granularity liquid-argon (LAr) sampling electromagnetic calorimeters. An iron-scintillator tile calorimeter provides hadronic coverage in the central rapidity range. The end-cap and forward regions are instrumented with LAr calorimetry for both electromagnetic and hadronic measurements. The muon spectrometer (MS) surrounds the calorimeters and consists of three large superconducting toroids, each with eight coils, a system of precision tracking chambers, and detectors for triggering.

The data used in this analysis were recorded in 2010 at the LHC at a centre-of-mass energy of 7 TeV . Application of beam, detector, and data-quality requirements results in a total integrated luminosity of 35 to $40 \mathrm{pb}^{-1}$ depending on the search channel, with an estimated uncertainty of $\pm 3.4 \%$ [17]. The events were triggered either by a single lepton or a pair of photon candidates with transverse momentum ( $p_{\mathrm{T}}$ ) thresholds which were significantly below the analysis offline requirements. The trigger introduces very little inefficiency except in one channel, $H \rightarrow$ $W W \rightarrow \ell \nu q q$, where there are efficiency losses in the muon channel of about $16 \%$.

Electron and photon candidates are reconstructed from energy clusters recorded in the liquid-argon electromagnetic calorimeter. The clusters must have shower profiles consistent with those expected from an electromagnetic shower. Electron candidates are matched to tracks reconstructed in the inner detector, while photon candidates require either no track or an identified conversion candidate. Muon candidates are reconstructed by matching tracks found in the inner detector with either tracks or hit segments in the muon spectrometer. Details of the quality criteria required on each of these objects differ amongst the analyses discussed here. There are in addition isolation criteria which again depend upon the specific backgrounds relevant to each analysis.

Jets are reconstructed from topological clusters [18] in the calorimeter using an anti- $\mathrm{k}_{\mathrm{t}}$ algorithm [19] with a radius parameter $R=0.4$. They are calibrated [18, 20] from the electromagnetic scale to the hadronic energy scale using $p_{\text {T }}$ and $\eta$ dependent correction factors based on Monte Carlo simulation and validated on data. They are required to have a $p_{\mathrm{T}}$ greater than 25 GeV unless otherwise stated. B tagging is performed using a secondary vertex algorithm based upon the decay length significance. A selection requirement is set to describe a jet as ' $b$-tagged' which has a $50 \%$ efficiency for true $b$-jets. The missing transverse energy is reconstructed

[^43]from topological energy clusters in the ATLAS calorimeters, with corrections for measured muons.

## 3 Cross sections, decays and simulation tools

### 3.1 Search for the standard model Higgs boson

At the LHC, the most important Standard Model Higgs boson production processes are the following four: gluon fusion $(g g \rightarrow H)$, which couples to the Higgs boson via a heavy-quark triangular loop; fusion of vector bosons radiated off quarks $(q q \rightarrow q q H)$; associated production with a vector boson $(q \bar{q} \rightarrow W H / Z H)$; associated production with a top-quark pair $(q \bar{q} / g g \rightarrow t \bar{t} H)$. The current calculations of the production cross sections have been gathered and summarised in Ref. [21].

Higher-order corrections have been calculated up to next-to-next-to-leading order (NNLO) in QCD for the gluon fusion [22-27], vector boson fusion [28] and associated $W H / Z H$ production processes [29], and to next-to-leading order (NLO) for the associated production with a $t \bar{t}$ pair [30, 31]. In addition, QCD soft-gluon resummations up to next-to-next-to-leading $\log$ (NNLL) are available for the gluon fusion process [32]. The NLO electroweak (EW) corrections are applied to the gluon fusion [33, 34], vector boson fusion [35, 36] and the associated $W H / Z H$ production [37] processes.

The Higgs boson decay branching ratios used take into account the recently calculated higher order QCD and EW corrections in each Higgs boson decay mode [21, 38]. The errors in these calculations for the states considered here are at most $2 \%$ and are neglected. For most four-fermion final states the predictions by Prophecy $4 \mathrm{f}[39,40]$ are used which include the complete NLO QCD+EW corrections with all interference and leading two-loop heavy Higgs boson corrections to the four-fermion width. The $H \rightarrow Z Z \rightarrow \ell \ell q q$ and $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ analyses use the less precise single $Z$ boson decay rates from Ref. [41].

The total signal production cross section in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$, multiplied by the branching ratio for the final states considered in this paper, is summarised in Fig. 1 as a function of the Higgs boson mass. Sources of uncertainties on these cross sections include missing higher-order corrections, imprecise knowledge of the parton distribution functions (PDFs) and the uncertainty on the strong force coupling constant, $\alpha_{s}$. These uncertainties are treated according to the recommendations given in Refs. [21, 42-45] and are $\pm(15-20) \%$ for the gluon fusion process, $\pm(3-9) \%$ for the vector boson fusion process and $\pm 5 \%$ for the associated $W H / Z H$ production process.


Fig. 1 The cross section multiplied by decay branching ratios for Standard Model Higgs boson production in $p p$ collisions at a 7 TeV cen-tre-of-mass energy as a function of mass [21]. All production modes are summed, and only final states considered in this paper are shown. Two bands are shown for each curve; the inner represents the QCD scale uncertainty and the outer also includes the $\alpha_{s}$ and PDF uncertainty

### 3.2 Higgs boson search in fourth generation models

Models with a fourth generation of heavy leptons and quarks with Standard Model-like couplings to the Higgs boson enhance its production cross section in gluon fusion by a factor of 4 to 10 compared to the predicted rate with three generations [46-49]. The model considered here [50] has very heavy fourth generation fermions, giving a minimum cross section but excluding the possibility that the Higgs boson decays to heavy neutrinos. These can weaken the exclusion for Higgs boson masses below the $W$ pair threshold [51]. It should be noted that the branching ratio into photons is suppressed by a factor around 8 in this model.

The Higgs boson production cross section in the gluon fusion process and its decay branching ratios have been calculated in the fourth generation model at NLO with HIGLU [52] and HDECAY [38]. The NNLO+NNLL QCD corrections are applied to the gluon fusion cross sections. The QCD corrections for the fourth generational model are assumed to be the same as in the Standard Model. The full two-loop Standard Model electroweak corrections [33, 34] are taken into account. The effect of a fourth generation in the Standard Model background processes, which includes contributions from loop diagrams, has been neglected.

### 3.3 Monte Carlo simulations

For the $H \rightarrow Z Z$ Monte Carlo samples, the Higgs signal is generated using PYTHIA [53] interfaced to PHOTOS [54] for final-state radiation. The $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ events produced by gluon fusion or vector boson fusion are modelled using the MC@NLO [55, 56] and SHERPA [57]

Monte Carlo generators, respectively. $H \rightarrow W W \rightarrow \ell v q q$ is modelled using PYTHIA for the gluon fusion and HERWIG [58] for vector boson fusion. The $\gamma \gamma$ signal is simulated with MC@NLO, HERWIG and PYTHIA for the gluon fusion, vector boson fusion and associated production processes respectively.

For background sample generation, the PYTHIA, ALPGEN [59], MC@NLO, MADGRAPH [60], SHERPA and HERWIG packages are employed.

All Monte Carlo samples are processed through a complete simulation of the ATLAS detector [61] using the GEANT programme [62].

## 4 Search for $H \rightarrow \gamma \gamma$

The search for the Higgs boson in the $\gamma \gamma$ decay mode is described below; further details can be found in Ref. [7]. The event selection requires the presence of at least two identified photons [63], including converted photons, isolated from any other activity in the calorimeter. The leading and the sub-leading photons are required to have transverse momenta above 40 GeV and 25 GeV , respectively. The directions of the photons are measured using the position determined in the first sampling of the electromagnetic calorimeter and that of the reconstructed primary vertex. The diphoton invariant mass spectrum is used to search for a peak above the background contributions.

The main background processes in the $H \rightarrow \gamma \gamma$ search arise from the production of two isolated prompt photons $(\gamma \gamma)$ and from fake photons in photon-jet ( $\gamma j$ ) and di-jet $(j j)$ events. Fake photons can originate from jets in which a leading $\pi^{0}$ or $\eta$ meson from the quark or gluon fragmentation is reconstructed as a single isolated photon. Each of these background contributions has been estimated from sideband control samples in the data. The backgroud from Drell-Yan events, $Z / \gamma^{*} \rightarrow e e$, where the electrons are mistakenly identified as photons, is estimated from studies of the $Z$ boson mass peak and extrapolated to the signal region. The total number of estimated background events is constrained to be the observed number. The di-photon invariant mass distribution for the events passing the full selection is shown in Fig. 2. The full-width at half maximum of a signal with $m_{h}=120 \mathrm{GeV}$ would be 4.2 GeV .

The expected signal yield, summing all production processes, and estimated background composition for a total integrated luminosity of $38 \mathrm{pb}^{-1}$ are summarised in Table 1. A total of 99 events passing all selection criteria are observed in data in the di-photon mass range from 100 GeV to 150 GeV . The background in this region is modelled by fitting an exponential function to the data. The signal peak is modelled by a Gaussian core portion and a power-law low-end tail [64]. Tails in the signal resolution are modelled


Fig. 2 Distribution of the di-photon invariant mass for the 99 events from data passing all event selection criteria in the $H \rightarrow \gamma \gamma$ search and for the Monte Carlo prediction. The overall uncertainty on the expected total yield is illustrated by the yellow band. The uncertainty due to the reducible background is also shown (dark yellow band). The predictions for the main components of the background (di-photon, pho-ton-jet, jet-jet and Drell-Yan) are also illustrated

Table 1 The number of expected and observed events in the $H \rightarrow \gamma \gamma$ search in the di-photon mass range from 100 GeV to 150 GeV for an integrated luminosity of $38 \mathrm{pb}^{-1}$. Also shown is the composition of the background expected from Monte Carlo simulation and the division of the observed data as discussed in the text as well as the expected number of $H \rightarrow \gamma \gamma$ signal events for a Higgs boson mass of $m_{H}=120 \mathrm{GeV}$. Total uncertainties are shown in the middle column while in the rightmost column the statistical and systematic uncertainties, respectively, are given

| Total | $\frac{\text { Expected }}{120 \pm 27}$ | $\frac{\text { Observed or Estimated }}{99}$ |
| :--- | :--- | :--- |
| $\gamma \gamma$ | $86 \pm 23$ | $75.0 \pm 13.3_{-3.6}^{+2.7}$ |
| $\gamma j$ | $31 \pm 15$ | $19.6 \pm 7.5 \pm 3.9$ |
| $j j$ | $1 \pm 1$ | $1.5 \pm 0.7_{-0.5}^{+1.8}$ |
| $Z / \gamma^{*}$ | $2.7 \pm 0.2$ | $2.9 \pm 0.1 \pm 0.6$ |
| $H \rightarrow \gamma \gamma$ | $0.45_{-0.10}^{+0.11}$ | $\left(m_{H}=120 \mathrm{GeV}\right)$ |

by a wide Gaussian component of small amplitude. No significant excess of events over the continuous background is found for any Higgs boson mass. The systematic uncertainty on the total signal acceptance is $\pm 15 \%$, where the dominant contributions come from photon identification $( \pm 11 \%)$ and photon isolation efficiencies $( \pm 10 \%)$.

## 5 Search for $\boldsymbol{H} \rightarrow \boldsymbol{W} \boldsymbol{W}$

The search for the Higgs boson in the decay channel $H \rightarrow W W$ benefits from the large branching ratio of the Higgs boson to decay into a pair of $W$ bosons for masses above $m_{H} \gtrsim 110 \mathrm{GeV}$, the sizable $W$ boson decay rates to leptons and the powerful identification of leptons with
the ATLAS detector. It offers the greatest sensitivity of any search channel when the Higgs boson mass is close to twice the $W$ boson mass, $m_{H} \sim 165 \mathrm{GeV}$. Two different decay modes of the $W$ bosons are considered: the $H \rightarrow W W^{*} \rightarrow \ell \nu \ell \nu$ channel is pursued for Higgs boson masses in the range from 120 GeV to 200 GeV , and the $H \rightarrow W W \rightarrow \ell \nu q q$ decay mode is used for Higgs boson masses in the range from 220 GeV to 600 GeV . The analyses are described below and further details can be found in Refs. [8, 9].

### 5.1 Search for $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$

The $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ analysis is performed using a dataset corresponding to an integrated luminosity of $35 \mathrm{pb}^{-1}$. Events are selected requiring exactly two isolated leptons with opposite charge. The leading lepton is required to have $p_{\mathrm{T}}>20 \mathrm{GeV}$ and the sub-leading lepton is required to have $p_{\mathrm{T}}>15 \mathrm{GeV}$. Events are classified into three channels depending on the lepton flavours: $e \mu$, $e e$ or $\mu \mu$. If the two leptons are of the same flavour, their invariant mass ( $m_{\ell \ell}$ ) is required to be above 15 GeV to suppress background from $\Upsilon$ production. To increase the sensitivity, the selections are then allowed to depend on the Higgs boson mass hypothesis. For all lepton combinations in the low (high) mass Higgs boson search, $m_{\ell \ell}$ is required to be below 50 (65) GeV for Higgs boson masses $m_{H} \leq 170 \mathrm{GeV}\left(m_{H}>170 \mathrm{GeV}\right)$ which suppress backgrounds from top-quark production and $Z$ boson production. The missing transverse energy in the event is required to be $E_{\mathrm{T}}^{\text {miss }}>30 \mathrm{GeV}$. An upper bound is imposed on the azimuthal angle between the two leptons, $\Delta \phi_{\ell \ell}<1.3$ (1.8) radians, taking advantage of the spin correlations [65] expected in the Higgs boson decay. The signal region is defined by the transverse mass $\left(m_{\mathrm{T}}\right)$ [66]:
$m_{\mathrm{T}}=\sqrt{\left(E_{\mathrm{T}}^{\ell \ell}+E_{\mathrm{T}}^{\mathrm{miss}}\right)^{2}-\left(\mathbf{P}_{\mathrm{T}}^{\ell \ell}+\mathbf{P}_{\mathrm{T}}^{\mathrm{miss}}\right)^{2}}$,
where $E_{\mathrm{T}}^{\ell \ell}=\sqrt{\left(\mathbf{P}_{\mathrm{T}}^{\ell \ell}\right)^{2}+m_{\ell \ell}^{2}},\left|\mathbf{P}_{\mathrm{T}}^{\mathrm{miss}}\right|=E_{\mathrm{T}}^{\mathrm{miss}}$ and $\mathbf{P}_{\mathrm{T}}^{\ell \ell}$ is the transverse momentum of the dilepton system. The transverse mass is required to be $0.75 \cdot m_{H}<m_{\mathrm{T}}<m_{H}$ for the event to be considered in a given $m_{H}$ range. Events are also treated separately depending on whether they have zero jets ( 0 -jet channel) or one jet (1-jet channel) reconstructed with $|\eta|<4.5$ due to the differences in background composition and expected signal-to-background ratio. To suppress background from top-quark production, events in the 1-jet channel are rejected if the jet is identified as coming from a $b$ quark. Events with two or more jets have been analysed as a separate channel. However, due to the marginal contribution to the overall sensitivity given the current total integrated luminosity and the additional systematic uncertainties, this channel is not included in this combination.

The expected background contributions from $W W$, topquark and $W+$ jets production are normalised using dedicated control regions in data as described in the next sections. Other smaller backgrounds are normalised according to their theoretical cross sections. The background from $Z / \gamma^{*}+$ jets production is normalised to the theoretical cross section with a correction factor determined from data.

### 5.1.1 The WW background

The di-boson $W W$ continuum can be distinguished from the Higgs boson signal through the kinematic selections. A control region is defined by changing the cut on $m_{\ell \ell}$ to require over 80 GeV (but not within 10 GeV of the $Z$ boson mass if the leptons are of the same flavour) and removing the selections on $m_{\mathrm{T}}$ and $\Delta \phi_{\ell \ell}$. The expected ratio of the background contribution in the control region and in the signal region is taken from Monte Carlo simulation. The three main sources of systematic uncertainty affecting this ratio are the theoretical uncertainty on the extrapolation, the jet energy scale uncertainty and the limited statistics in the simulated sample. Uncertainties due to these effects of $\pm 6 \%$ in the 0 -jet channel and $\pm 17 \%$ in the 1-jet channel have been determined.

### 5.1.2 The $t \bar{t}$ and single top-quark backgrounds

Top-quarks, whether from strong interaction $t \bar{t}$ production or weak interaction single top-quark production, are a copious source of final states with one or two $W$ bosons accompanied by one or more jets. Due to kinematic selection one or more of these jets may fail identification, thereby leading to a final state similar to that from the $H \rightarrow W W$ signal.

The background from top-quark production in the 0 -jet channel is estimated by first removing the jet veto. This gives a sample dominated by top-quarks, and the expected contamination from other processes in the control region is subtracted from the observed event yield. Then the probability that top events pass the jet veto is derived from the measured probability of not reconstructing a jet in data, using a sample of top candidates with two leptons, one b-jet and no other jet. The dominant systematic uncertainties originate from the limited statistics in data and the jet energy scale. A total uncertainty of $\pm 60 \%$ has been determined for the top-quark background estimate in the 0 -jet channel.

The top-quark background in the 1 -jet channel is normalised using a control region where the veto on jets coming from $b$-quarks is reversed and the $\Delta \phi_{\ell \ell}, m_{\ell \ell}$ and $m_{\mathrm{T}}$ selections are removed. An extrapolation factor from the control region to the signal region is estimated from Monte Carlo simulation. The dominant systematic uncertainties on the top-quark background estimate in the 1-jet channel are $\pm 23 \%$ from the theoretical uncertainties on the extrapolation factor and $\pm 22 \%$ from the uncertainty on the $b$-tagging efficiency.

### 5.1.3 The $W+$ jets background

The production of $W$ bosons accompanied by jets can mimic the $H \rightarrow W W$ signal if one of the jets is mis-identified as an isolated lepton. The $W+$ jets background is normalised using a control region defined by relaxing the identification and isolation criteria for one of the two leptons. The contribution to the signal region is estimated by multiplying the rate measured in the control region by the probability for fake leptons which pass the relaxed identification and isolation criteria to also pass the original lepton selection criteria. This misidentification probability is measured in a multi-jet data sample. The major sources of systematic uncertainty for the $W+$ jets background estimate come from the bias introduced by the jet trigger threshold used to select the multi-jet events and the residual difference in kinematics and flavour composition of the jets in multi-jet events and in events from $W+$ jets production. The total uncertainty on the estimated $W+$ jets background is $\pm 50 \%$.

### 5.1.4 The $Z / \gamma^{*}+$ jets background

The largest cross section for producing two isolated, high$p_{\mathrm{T}}$ leptons comes from the $Z / \gamma^{*} \rightarrow \ell \ell$ process. The background from $Z / \gamma^{*}+$ jets is significantly reduced by the upper bound on $m_{\ell \ell}$ and the requirement of high $E_{\mathrm{T}}^{\text {miss }}$ in the signal region. To correct for potential mis-modelling of the distribution of $E_{\mathrm{T}}^{\mathrm{miss}}$ at high values, a correction factor is derived from the observed difference between the fraction of events passing the $E_{\mathrm{T}}^{\text {miss }}>30 \mathrm{GeV}$ selection in data and Monte Carlo simulation for events with $m_{\ell \ell}$ within 10 GeV of the $Z$ boson mass [41]. As the discrepancy between data and Monte Carlo tends to be larger in events with jets, the correction factor is larger in the 1 -jet channel than in the 0 -jet channel. The flavours of the two leptons in the event also impact the magnitude of the correction factor, since any discrepancies between data and simulation have different sources. In the 1-jet channel, the correction factors are found to be $1.2 \pm 0.4 \pm 0.1^{3}$ in the $e e$ analysis and $2.4 \pm 0.5 \pm 0.2$ in the $\mu \mu$ analysis. Under the assumption that the same correction factors apply to events below the upper bound on $m_{\ell \ell}$, the expected $Z / \gamma^{*}+$ jets background is obtained from the Monte Carlo simulation normalised to the product of the theoretical cross section and the correction factors.

### 5.1.5 Results for the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ search

The expected and observed numbers of events in the $H \rightarrow$ $W W$ analysis for a Higgs boson mass of 170 GeV are shown in Table 2. Three events in total are observed in the 0 -jet

[^44]Table 2 Numbers of expected signal ( $m_{H}=170 \mathrm{GeV}$ ) and background events and the observed numbers of events in the data passing all selections in the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ search. The dataset used in this analysis corresponds to an integrated luminosity of $35 \mathrm{pb}^{-1}$. The uncertainties shown are the statistical and systematic uncertainties respectively

|  | $e \mu$ | $e e$ | $\mu \mu$ |
| :--- | :--- | :--- | :--- |
| 0 -jet channel |  |  |  |
| $W W$ | $0.71 \pm 0.05 \pm 0.06$ | $0.20 \pm 0.03 \pm 0.02$ | $0.53 \pm 0.02 \pm 0.05$ |
| $t \bar{t}$ and single top | $0.09 \pm 0.05 \pm 0.06$ | $0.03 \pm 0.01 \pm 0.02$ | $0.08 \pm 0.04 \pm 0.06$ |
| $W Z / Z Z / W \gamma$ | $0.020 \pm 0.001 \pm 0.001$ | $0(<0.001) \pm 0$ | $0.010 \pm 0.001 \pm 0.001$ |
| $Z / \gamma^{*}+$ jets | $0(<0.001) \pm 0$ | $0(<0.001) \pm 0$ | $0(<0.002) \pm 0$ |
| $W+$ jets | $0.01 \pm 0.01 \pm 0.01$ | $0.02 \pm 0.01 \pm 0.01$ | $0 \pm 0.10 \pm 0.01$ |
| Total Background | $0.83 \pm 0.07 \pm 0.13$ | $0.25 \pm 0.08 \pm 0.04$ | $0.62 \pm 0.05 \pm 0.10$ |
| $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ | $0.62 \pm 0.01 \pm 0.18$ | $0.20 \pm 0.01 \pm 0.07$ | $0.44 \pm 0.01 \pm 0.12$ |
| Observed | 1 | 1 | 1 |
| 1 -jet channel |  |  |  |
| $W W$ | $0.18 \pm 0.03 \pm 0.03$ | $0.05 \pm 0.02 \pm 0.01$ | $0.16 \pm 0.03 \pm 0.02$ |
| $t \bar{t}$ and single top | $0.26 \pm 0.07 \pm 0.11$ | $0.10 \pm 0.02 \pm 0.04$ | $0.15 \pm 0.04 \pm 0.07$ |
| $W Z / Z Z / W \gamma$ | $0.01 \pm 0.001 \pm 0.001$ | $0(<0.001) \pm 0$ | $0(<0.001) \pm 0$ |
| $Z / \gamma^{*}+$ jets | $0(<0.01) \pm 0$ | $0.05 \pm 0.02 \pm 0.02$ | $0.25 \pm 0.08 \pm 0.05$ |
| $W+$ jets | $0.02 \pm 0.02 \pm 0.01$ | $0.03 \pm 0.20 \pm 0.01$ | $0 \pm 0.10 \pm 0.01$ |
| Total Background | $0.47 \pm 0.08 \pm 0.16$ | $0.23 \pm 0.04 \pm 0.06$ | $0.56 \pm 0.09 \pm 0.14$ |
| $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ | $0.31 \pm 0.01 \pm 0.09$ | $0.08 \pm 0.01 \pm 0.03$ | $0.21 \pm 0.01 \pm 0.06$ |
| Observed | 0 | 0 | 1 |

channel for the combined $e e, e \mu$ and $\mu \mu$ final states, compared to an expected number of events from background sources only of $1.70 \pm 0.12 \pm 0.17$. More events are expected in the $\mu \mu$ channel compared to the $e e$ channel due to different lepton identification efficiencies for electrons and muons. In the 1 -jet channel, one event is observed in the data compared to a total number of expected events from background sources of $1.26 \pm 0.13 \pm 0.23$. The observed $m_{\mathrm{T}}$ distributions in data after all selections except the transverse mass cut for the combined $e \mu, e e$ and $\mu \mu$ channels are compared to the expected distributions from simulated events in Fig. 3.

### 5.2 Search for $H \rightarrow W W \rightarrow \ell \nu q q$

The $H \rightarrow W W \rightarrow \ell \nu q q$ analysis uses a dataset corresponding to an integrated luminosity of $35 \mathrm{pb}^{-1}$. Events are selected requiring exactly one lepton with $p_{\mathrm{T}}>30 \mathrm{GeV}$. The missing transverse energy in the event is required to be $E_{\mathrm{T}}^{\mathrm{miss}}>30 \mathrm{GeV}$. Events with fewer than two jets are rejected. ${ }^{4}$ Events with $\geq 4$ jets are treated as a separate search channel, which is however not included in the current combination. The pair of jets with invariant mass closest to the $W$ boson mass is considered to be coming from the $W$ boson and the measured mass must be between 71 GeV and

[^45]91 GeV . The event is rejected if any of the jets in the event is identified as coming from a $b$-quark. The invariant mass of the Higgs boson candidate, $m_{\ell \nu q q}$, is reconstructed with a $W$ boson mass constraint on the lepton-neutrino system giving rise to a quadratic equation. If there are two solutions the one corresponding to the lower longitudinal momentum is taken; if complex the real part is used.

The dominant source of background events in the $H \rightarrow$ $W W \rightarrow \ell \nu q q$ search comes from $W+$ jets production. The contribution from QCD events is estimated by fitting the observed $E_{\mathrm{T}}^{\text {miss }}$ distribution as the sum of templates taken from simulation. Table 3 shows the expected numbers of signal and background events in the signal region, as well as the observation. In the channel with only two and no additional jets, 450 events are observed in the data passing all selection criteria compared to an expected yield from background sources of $450 \pm 41$ events. In the channel with one extra jet 263 events are observed, compared to an expected number of background events of $224 \pm 15$.

The distributions of the invariant mass for the Higgs boson candidates in data are compared to the expected distributions from simulated events in Fig. 4. The $m_{\ell \nu q q}$ background spectrum is modelled with a falling exponential function. The impact of the functional form has been investigated by replacing the single exponential with a double exponential, by histograms taken from simulation, and by a mixture of both methods without significant change in the results. It should be noted that the limit extraction is made using the
exponential fit, not by comparison with the simulated background.


Fig. 3 Distributions of the transverse mass $m_{\mathrm{T}}$ in the 0 -jet channel (a) and 1-jet channel (b) for the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ search after all selections except the transverse mass cut for the combined $e \mu$, ee and $\mu \mu$ channels. The error bars reflect Poisson asymmetric errors. A Higgs boson signal is shown for $m_{H}=170 \mathrm{GeV}$. The selections applied for $m_{H}=170 \mathrm{GeV}$ are indicated by the two vertical dotted lines


Fig. 4 Distributions of the invariant mass $m_{\ell v q q}$ for the $H \rightarrow W W \rightarrow \ell \nu q q$ search after the application of all selection criteria and the W-mass constrained fit. The background fit is shown as a continuous line. In (a) no extra jets are allowed and in (b) one additional jet is required. The Higgs boson signal is shown for $m_{H}=400 \mathrm{GeV}$ and the expected yield is scaled up by a factor of 30 for illustration purposes

Table 3 Numbers of expected signal $\left(m_{H}=400 \mathrm{GeV}\right)$ and background events and the observed numbers of events in the data passing all selections in the $H \rightarrow W W \rightarrow \ell \nu q q$ search. The dataset used corresponds to an integrated luminosity of $35 \mathrm{pb}^{-1}$. The quoted uncertainties are combinations of the statistical and systematic uncertainties

| $m_{H}=400 \mathrm{GeV}$ | $H+0$-jets |  |  | $H+1-\mathrm{jet}$ |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
|  | $e \nu q q$ |  | $\mu \nu q q$ |  | $e \nu q q$ |

## 6 Search for $\boldsymbol{H} \rightarrow \boldsymbol{Z} Z^{(*)}$

Three different $H \rightarrow Z^{(*)}$ final states are considered here: $H \rightarrow Z^{(*)} \rightarrow \ell \ell \ell \ell, H \rightarrow Z Z \rightarrow \ell \ell \nu v$ and $H \rightarrow Z Z \rightarrow$ $\ell \ell q q$. In the $H \rightarrow Z Z^{(*)} \rightarrow$ l८८८ search, the excellent energy and momentum resolutions of the ATLAS detector for electrons and muons lead to a narrow expected four-lepton invariant mass peak on top of a continuous background. The dominant background component is the irreducible $\mathrm{ZZ}^{(*)} \rightarrow$ lell process. In the low Higgs boson mass region, where one of the $Z$ bosons is off-shell and decays into a pair of low transverse momentum leptons, the reducible backgrounds from $Z+$ jets production and $t \bar{t}$ production are also important. For Higgs boson masses above $m_{H} \gtrsim 200 \mathrm{GeV}$ both $Z$ bosons are on-shell. In this region the decay modes $H \rightarrow Z Z \rightarrow \ell \ell q q$ and $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$, which have substantially larger branching ratios but also larger backgrounds compared to the $H \rightarrow Z Z^{(*)} \rightarrow \ell \ell \ell \ell$ decay, provide additional sensitivity. The analyses of the $H \rightarrow Z Z \rightarrow \ell \ell q q$ and $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ channels require that both $Z$ bosons are on-shell, which limits the contribution from the reducible backgrounds from $Z+$ jets production and $t \bar{t}$ production. In this paper the $H \rightarrow Z Z \rightarrow \ell \ell q q$ and $H \rightarrow Z Z \rightarrow \ell \ell \nu v$ search channels have been used for Higgs boson masses in the range $200 \mathrm{GeV} \leq m_{H} \leq 600 \mathrm{GeV}$, a range extending beyond the sensitivities of LEP and Tevatron experiments [4, 6]. Further details of the three analyses can be found in Refs. [10, 11].

### 6.1 Search for $H \rightarrow Z^{(*)} \rightarrow$ lौौौ

Candidate events are selected requiring two same-flavour and opposite-charge pairs of leptons. Muons with $p_{\mathrm{T}}>7 \mathrm{GeV}$ and electrons with $p_{\mathrm{T}}>15 \mathrm{GeV}$ are considered, while at least two out of the four leptons must satisfy $p_{\mathrm{T}}>20 \mathrm{GeV}$. All leptons are required to be well separated from each other, isolated from other activity in the tracking detectors and the calorimeters and have low track impact parameters with respect to the primary vertex. At least one of the lepton pairs is required to have an invariant mass within 15 GeV (within 12 GeV if the combined four-lepton mass is high) of the $Z$ boson mass. The requirement on the invariant mass of the second lepton pair varies as a function of the Higgs boson candidate mass, $m_{\ell \ell \ell \ell}$. The effective Higgs boson candidate mass resolution $\sigma\left(m_{H}\right)$, including the intrinsic width at the Higgs boson mass hypothesis being tested, is used to define an allowed range for the reconstructed Higgs boson candidate mass. The latter is required to be within $\pm 5 \sigma\left(m_{H}\right)$ of the tested Higgs boson mass for the event to be considered.

The magnitude of the $Z Z^{(*)}$ background is normalised to the measured $Z$ boson cross section multiplied by the expected ratio of the cross sections $\sigma_{Z Z} / \sigma_{Z}$ from theoretical
calculations [67]. This estimate is independent of the luminosity uncertainty, and the cross section ratio is less affected by theoretical uncertainties than the $\sigma_{Z Z}$ cross section alone. The total uncertainty on the $Z Z^{(*)}$ background estimate is $\pm 15 \%$. The reducible $Z+$ jets background arises predominantly from $Z$ boson production in association with a pair of heavy flavour quarks which decay semi-leptonically. This background is normalised using dedicated control regions in data where the lepton identification requirements are relaxed for the second pair of leptons. The final uncertainty on the $Z+$ jets background is $\pm 20 \%$. The $t \bar{t}$ background is estimated from Monte Carlo simulation and normalised to its theoretical cross section. A total uncertainty of $\pm 25 \%$ is estimated for the $t \bar{t}$ background contribution.

After the application of all selection criteria, no candidate events remain in data for the $H \rightarrow Z^{(*)} \rightarrow \ell \ell \ell \ell$ search at any Higgs boson mass. This is consistent with the small background and signal yields expected with the integrated luminosity of $40 \mathrm{pb}^{-1}$ used in this analysis. The results are shown in Table 4 for two selected Higgs boson masses of $m_{H}=130 \mathrm{GeV}$ and $m_{H}=200 \mathrm{GeV}$. The distribution of the Higgs boson candidate invariant mass, $m_{\ell \ell \ell \ell}$, before applying the lepton impact parameter and isolation requirements is shown in Fig. 5.

Table 4 Expected signal and background event yields in the $H \rightarrow$ $Z Z^{(*)} \rightarrow$ € $\ell \ell$ search within $\pm 5 \sigma\left(m_{H}\right)$ for two selected Higgs boson masses. No events are observed in the data. The dataset used corresponds to a total integrated luminosity of $40 \mathrm{pb}^{-1}$. The quoted uncertainties are combinations of the statistical and systematic uncertainties

| $m_{H}(\mathrm{GeV})$ | 130 | 200 |
| :--- | :--- | :--- |
| Total background | $0.010 \pm 0.002$ | $0.090 \pm 0.014$ |
| $H \rightarrow Z^{(*)} \rightarrow$ eौe८ | $0.015 \pm 0.003$ | $0.095 \pm 0.017$ |
| Observed | 0 | 0 |



Fig. 5 Distribution of $m_{\ell \ell \ell \ell}$ in the $H \rightarrow Z Z^{(*)} \rightarrow$ थौौौ search before applying the lepton impact parameter and isolation requirements which remove the two candidates. The error bars reflect Poisson asymmetric errors
6.2 Search for $H \rightarrow Z Z \rightarrow \ell \ell q q$

Events are selected requiring exactly two same-flavour leptons with an invariant mass $76 \mathrm{GeV}<m_{\ell \ell}<106 \mathrm{GeV}$ and at least two jets. To reduce background from top production the missing transverse energy is required to be $E_{\mathrm{T}}^{\mathrm{miss}}<$ 50 GeV . The two jets in the event with the highest individual $p_{\mathrm{T}}$ are required to have an invariant mass, $m_{j j}$, in the range $70 \mathrm{GeV}<m_{j j}<105 \mathrm{GeV}$. Additional background rejection is obtained for high mass by using the fact that the final state jets and leptons are boosted in the directions of the two $Z$ bosons. For Higgs boson searches at $m_{H} \geq 360 \mathrm{GeV}$, the two jets are required to have $p_{\mathrm{T}}>50 \mathrm{GeV}$. Furthermore, the azimuthal angles between the two jets, $\Delta \phi_{j j}$, and between the two leptons, $\Delta \phi_{\ell \ell}$, must both be less than $\pi / 2$.

The Higgs boson candidate mass is constructed from the invariant mass of the two leptons and the two jets in the event, $m_{\ell \ell j j}$. The two jets are constrained to have an invariant mass equal to the $Z$ boson mass to improve the Higgs boson candidate mass resolution.

### 6.2.1 Background estimates for the $H \rightarrow Z Z \rightarrow \ell \ell q q$ search

The dominant background in the $H \rightarrow Z Z \rightarrow \ell \ell q q$ search channel is expected to come from $Z+$ jets production. Other significant sources are $t \bar{t}$ production, multi-jet production and $Z Z / W Z$ production. All backgrounds, except for the multi-jet background, are estimated from Monte Carlo simulation. For the $Z+$ jets and the $t \bar{t}$ backgrounds the predictions from simulation are compared against data in control samples which are dominated by these backgrounds. The $Z+$ jets control region is defined by modifying the $m_{j j}$ selection to instead require $40 \mathrm{GeV}<m_{j j}<70 \mathrm{GeV}$ or $105 \mathrm{GeV}<m_{j j}<150 \mathrm{GeV}$. The $t \bar{t}$ control region is defined by reversing the $E_{\mathrm{T}}^{\text {miss }}$ selection and modifying the $m_{\ell \ell}$ selection to require $60 \mathrm{GeV}<m_{\ell \ell}<76 \mathrm{GeV}$ or $106 \mathrm{GeV}<$ $m_{\ell \ell}<150 \mathrm{GeV}$. Both the $Z+$ jets and the $t \bar{t}$ background estimates from Monte Carlo simulation are found to be in
good agreement with data in the control samples. The contribution from $W+$ jets is very small and assumed to be adequately modelled. The multi-jet background in the electron channel is derived from a sample where the electron identification requirements are relaxed. In the muon channel, the multi-jet background is taken from Monte Carlo after verifying the accuracy of the simulation using a data sample where the two muons in the event are required to have the same charge.

### 6.2.2 Results for the $H \rightarrow Z Z \rightarrow \ell$ €qq search

The $H \rightarrow Z Z \rightarrow \ell \ell q q$ analysis is performed for Higgs boson masses between 200 GeV and 600 GeV in steps of 20 GeV . Table 5 summarises the numbers of estimated background events and observed events in data for the selections below and above $m_{H}=360 \mathrm{GeV}$. The numbers of expected signal events for two representative Higgs boson masses are also shown. For the low mass search, 216 events are observed in data passing all selection criteria compared to an expected number of events from background sources only of $226 \pm 4 \pm 28$ events. The corresponding numbers for the high mass searches are 11 events observed in data compared to an expected yield of $9.9 \pm 0.9 \pm 1.5$ events from background sources only. The distribution of the reconstructed Higgs boson candidate mass $m_{\ell \ell j j}$ for the events passing all of the selection criteria is shown in Fig. 6.

### 6.3 Search for $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$

The $H \rightarrow Z Z \rightarrow \ell \ell \nu v$ final state is characterised by two charged leptons and large $E_{\mathrm{T}}^{\text {miss }}$. Events are selected by requiring exactly two leptons of the same flavour with an invariant mass $76 \mathrm{GeV}<m_{\ell \ell}<106 \mathrm{GeV}$. Events are rejected if any jet is identified as coming from a $b$-quark. The selection has been optimised separately for searches at low ( $m_{H}<280 \mathrm{GeV}$ ) and high ( $m_{H} \geq 280 \mathrm{GeV}$ ) values of the Higgs boson mass. Events are required to have $E_{\mathrm{T}}^{\text {miss }}>66(82) \mathrm{GeV}$ and $\Delta \phi_{\ell \ell}<2.64$ (2.25) radians for

Table 5 Numbers of events estimated as background, observed in data and expected from signal in the
$H \rightarrow Z Z \rightarrow \ell \ell q q$ search for low mass ( $m_{H}<360 \mathrm{GeV}$ ) and high mass ( $m_{H} \geq 360 \mathrm{GeV}$ ) selections. The signal, quoted at two mass points, includes small contributions from llll and $\ell \ell \nu v$ decays. Electron and muon channels are combined. The uncertainties shown are the statistical and systematic uncertainties, respectively

| Source | Low mass selection | High mass selection |
| :--- | :--- | :--- |
| $Z+$ jets | $214 \pm 4 \pm 27$ | $9.1 \pm 0.9 \pm 1.4$ |
| $W+$ jets | $0.33 \pm 0.16 \pm 0.17$ | - |
| $t \bar{t}$ | $0.94 \pm 0.09 \pm 0.25$ | $0.08 \pm 0.02 \pm 0.03$ |
| Multi-jet | $3.81 \pm 0.65 \pm 1.91$ | $0.11 \pm 0.11 \pm 0.06$ |
| $Z Z$ | $3.80 \pm 0.10 \pm 0.73$ | $0.30 \pm 0.03 \pm 0.06$ |
| $W Z$ | $2.83 \pm 0.05 \pm 0.88$ | $0.29 \pm 0.02 \pm 0.10$ |
| Total background | $226 \pm 4 \pm 28$ | $9.9 \pm 0.9 \pm 1.5$ |
| $H \rightarrow Z Z \rightarrow \ell \ell q q$ | $0.60 \pm 0.01 \pm 0.12\left(m_{H}=200 \mathrm{GeV}\right)$ | $0.24 \pm(<0.001) \pm 0.05\left(m_{H}=400 \mathrm{GeV}\right)$ |
| Observed | 216 | 11 |



Fig. 6 Distribution of $m_{\ell \ell j j}$ for events passing all of the selection criteria in the $H \rightarrow Z Z \rightarrow \ell \ell q q$ search. The expected yield for a Higgs boson with a mass $m_{H}=300 \mathrm{GeV}$ is also shown, multiplied by a factor of 20 for illustrative purposes. The contribution labelled "Other" is mostly from top events but includes also QCD multijet production
the low (high) mass region. For the low mass region $\Delta \phi_{\ell \ell}>$ 1 radian is also required. The Higgs boson candidate transverse mass is obtained from the invariant mass of the two leptons and the missing transverse energy.

### 6.3.1 Background estimates for the $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ search

A major background in the $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ search channel comes from di-boson production and is estimated from Monte Carlo simulation. Background contributions from $t \bar{t}$ and $W+$ jets production are also obtained from Monte Carlo simulation, and the estimated yields are verified by comparing with the number of observed events in dedicated control samples in the data. Both the $t \bar{t}$ and the $W+$ jets con-

Table 6 Numbers of events estimated from background, observed in data and expected from signal in the $H \rightarrow Z Z \rightarrow \ell \ell \nu v$ search for low mass ( $m_{H}<280 \mathrm{GeV}$ ) and high mass ( $m_{H} \geq 280 \mathrm{GeV}$ ) selections. Electron and muon channels are combined. The expected signal events
trol regions are defined by modifying the $m_{\ell \ell}$ selection to instead require $60 \mathrm{GeV}<m_{\ell \ell}<76 \mathrm{GeV}$ or $106 \mathrm{GeV}<$ $m_{\ell \ell}<150 \mathrm{GeV}$. The $t \bar{t}$ control region also requires that the events pass $E_{\mathrm{T}}^{\text {miss }}>20 \mathrm{GeV}$ and that at least one jet is identified as coming from a $b$-quark. The $W+$ jets control region instead requires $E_{\mathrm{T}}^{\text {miss }}>36 \mathrm{GeV}$ and that no jets in the events are identified as coming from a $b$-quark. The observed event yields in the control regions for $t \bar{t}$ and $W+$ jets production are in good agreement with the predictions from the Monte Carlo simulation. The background from $Z+$ jets production is estimated from Monte Carlo simulation after comparison studies of the $E_{\mathrm{T}}^{\text {miss }}$ distribution between Monte Carlo and data. The multi-jet background in the electron channel is derived from a sample where the electron identification requirements are relaxed. In the muon channel, the multi-jet background is estimated from a simulated sample of semi-leptonically decaying $b$ - and $c$-quarks and found to be negligible after the application of the $m_{\ell \ell}$ selection. This was verified in data using leptons with identical charges.

### 6.3.2 Results for the $H \rightarrow Z Z \rightarrow \ell \ell \nu v$ search

The $H \rightarrow Z Z \rightarrow \ell \ell \nu v$ analysis is performed for Higgs boson masses between 200 GeV and 600 GeV in steps of 20 GeV . Table 6 summarises the numbers of events observed in the data, the estimated numbers of background events and the expected numbers of signal events for two selected $m_{H}$ values. For the low mass selections, five events are observed in data compared to an expected number of events from background sources only of $5.8 \pm 0.5 \pm 1.3$. The corresponding results for the high mass selections are five events observed in data compared to an expected yield of $3.5 \pm 0.4 \pm 0.8$ events from background sources only. In addition to the $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ decays, several other Higgs boson channels give a non-negligible contribution to
include minor additional contributions from $H \rightarrow Z Z \rightarrow \ell \ell q q, H \rightarrow$ $Z Z^{(*)} \rightarrow \ell \ell \ell \ell$ and one which can be large from $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$. The uncertainties shown are the statistical and systematic uncertainties, respectively

| Source | Low mass selection | High mass selection |
| :--- | :--- | :--- |
| $Z+$ jets | $1.09 \pm 0.29 \pm 0.59$ | $1.01 \pm 0.29 \pm 0.58$ |
| $W+$ jets | $1.07 \pm 0.31 \pm 0.64$ | $0.41 \pm 0.19 \pm 0.22$ |
| $t \bar{t}$ | $1.90 \pm 0.10 \pm 0.63$ | $0.91 \pm 0.07 \pm 0.31$ |
| Multi-jet | $0.11 \pm 0.11 \pm 0.06$ | - |
| $Z Z$ | $0.58 \pm 0.01 \pm 0.11$ | $0.51 \pm 0.01 \pm 0.10$ |
| $W Z$ | $0.57 \pm 0.01 \pm 0.10$ | $0.45 \pm 0.01 \pm 0.09$ |
| $W W$ | $0.43 \pm 0.02 \pm 0.09$ | $0.16 \pm 0.01 \pm 0.04$ |
| Total background | $5.8 \pm 0.5 \pm 1.3$ | $3.5 \pm 0.4 \pm 0.8$ |
| $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ | $0.19 \pm(<0.001) \pm 0.04\left(m_{H}=200 \mathrm{GeV}\right)$ | $0.30 \pm(<0.001) \pm 0.06\left(m_{H}=400 \mathrm{GeV}\right)$ |
| Observed | 5 | 5 |

the total expected signal yield. In particular, $H \rightarrow W W^{(*)} \rightarrow$ $\ell \nu \ell \nu$ decays can lead to final states that are very similar to $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ decays. They are found to contribute significantly to the signal yield at low $m_{H}$ values. The expected number of events from $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ decays relative to that from $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ decays is $76 \%$ for $m_{H}=200 \mathrm{GeV}$ and $9 \%$ for $m_{H}=300 \mathrm{GeV}$. The kinematic selections prevent individual candidates from being accepted by both searches. The $E_{\mathrm{T}}^{\text {miss }}$ distribution before vetoing events with low $E_{\mathrm{T}}^{\text {miss }}$ is shown in Fig. 7.


Fig. 7 Distribution of missing transverse energy in the $H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ search in the electron channel before vetoing events with low $E_{\mathrm{T}}^{\text {miss }}$. The expected yield for a Higgs boson with $m_{H}=400 \mathrm{GeV}$ is also shown. The distribution in the muon channel is similar with four events seen which have $E_{\mathrm{T}}^{\text {miss }}$ above 80 GeV

Table 7 Summary of systematic uncertainties (in percent) of the signal yield. The correlated systematic uncertainties are given in detail, the uncorrelated ones are lumped together. The uncertainties are evaluated for a Higgs boson mass of 115 GeV for the $H \rightarrow \gamma \gamma$ channel, 160 GeV for $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu, 200 \mathrm{GeV}$ for the $H \rightarrow Z Z^{(*)} \rightarrow$ lell and 400 GeV for the remaining channels. Systematic errors

## 7 Combination method

The limit-setting procedure uses the power-constrained profile likelihood method known as the Power Constrained Limit, PCL [13, 14, 68]. This method is preferred to the more familiar $\mathrm{CL}_{s}[15]$ technique because the constraint is more transparently defined and it has reduced overcoverage resulting in a more precise meaning of the quoted confidence level. The resulting PCL median limits have been found to be around $20 \%$ tighter than those obtained with the $\mathrm{CL}_{s}$ method in several Higgs searches. The application of the PCL method to each of the individual Higgs boson search channels is described in Refs. [7-11]. A similar procedure is used here. The individual analyses are combined by maximising the product of the likelihood functions for each channel and computing a likelihood ratio. A single signal normalisation parameter $\mu$ is used for all analyses, where $\mu$ is the ratio of the hypothesised cross section to the expected Standard Model cross section.

Each channel has sources of systematic uncertainty, some of which are common with other channels. Table 7 lists the common sources of systematic uncertainties, which are taken to be $100 \%$ correlated with other channels. Let the search channels be labelled by $l(l=H \rightarrow \gamma \gamma, H \rightarrow W W$, $\ldots$ ), the background contribution, $j$, to channel $l$ by $j_{l}$ and the systematic uncertainties by $i$ ( $i=$ luminosity, jet energy scale, ...). The relative magnitude of the effect on the Higgs boson signal yield in channel $l$ due to systematic uncertainty $i$ is then denoted by $\epsilon_{l i}^{s}$, and on background contribution $j_{l}$, $\epsilon_{j l i}^{b}$. The $\epsilon_{l i}$ 's are constants; an individual $\epsilon_{l i}^{s}$ can be zero
marked with a dash are neglected. In the three channels, the impact of the lepton energy scale and resolution uncertainties on the efficiency was found to be negligible, but they can still influence the fit via the signal distributions. In the $H \rightarrow W W \rightarrow \ell v q q$ channel a jet energy scale uncertainty can only decrease the efficiency; the resolution uncertainty is negligible in comparison

|  | $\gamma \gamma$ | $\underline{H \rightarrow W W}$ |  | $\underline{H \rightarrow Z Z}$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | ८v $\ell \nu$ | $\ell \nu q q$ | lel¢ | $\ell \ell \nu$ | $\ell \ell q q$ |
| Luminosity | $\pm 3.4$ | $\pm 3.4$ | $\pm 3.4$ | $\pm 3.4$ | $\pm 3.4$ | $\pm 3.4$ |
| e/ $\gamma$ efficiency | $\pm 11$ | $\pm 8.2$ | $\pm 2.6$ | $\pm 2.1$ | $\pm 4.6$ | $\pm 0.0$ |
| $\mathrm{e} / \gamma$ energy scale | - | $\pm 1.6$ | - | - | $\pm 0.5$ | $\pm 0.2$ |
| $\mathrm{e} / \gamma$ resolution | - | $\pm 1.6$ | - | - | $\pm 0.1$ | $\pm 0.1$ |
| $\mu$ efficiency | - | $\pm 0.5$ | $\pm 1.0$ | $\pm 0.8$ | $\pm 0.0$ | $\pm 2.0$ |
| $\mu$ energy scale | - | $\pm 4.8$ | - | - | $\pm 1.2$ | ${ }_{-2.2}^{+0.2}$ |
| $\mu$ resolution | - | $\pm 1.2$ | - | - | $\pm 0.1$ | $\pm 0.1$ |
| Jet energy scale | - | $\pm 3.7$ | -26 | - | $\pm 0.4$ | ${ }_{-7.0}^{+2.9}$ |
| Jet energy resolution | - | - | - | - | $\pm 0.2$ | ${ }_{-1.3}^{+0.0}$ |
| $b$-tag efficiency | - | - | - | - | $\pm 0.4$ | - |
| Uncorrelated | $\pm 10$ | $\pm 5.0$ | - | - | - | - |

if the channel in question is not affected by this source of systematic uncertainty. A common systematic uncertainty, i, which is shared between channels $l$ and $l^{\prime}$ implies that $\epsilon_{l i}^{s}$ and $\epsilon_{l^{\prime} i}^{s}$ are both different from zero. If a systematic source $i$ is shared between the signal in channel $l$ and background contribution $j_{l}$ then both $\epsilon_{l i}^{s}$ and $\epsilon_{j l i}^{b}$ are non-zero. For each source of systematic uncertainty $i$ there is a corresponding nuisance parameter $\delta_{i}$ and an associated auxiliary measurement $m_{i}$ on a control sample (e.g. sidebands in a mass spectrum) that is used to constrain the parameter. The $\delta_{i}$ and $m_{i}$ are scaled so that $\delta_{i}=0$ corresponds to the nominal expectation and $\delta_{i}= \pm 1$ corresponds to the $\pm 1 \sigma$ variations of the source. When constructing ensembles for statistical evaluation, each $m_{i}$ is sampled according to $G\left(m_{i} \mid \delta_{i}, 1\right)$, the standard normal distribution. Using this notation, the total number of expected events in the signal region for channel $l$ is given by:

$$
\begin{align*}
N_{l}^{\exp }= & \mu L \sigma_{l} \prod_{i}\left(1+\epsilon_{l i}^{s} \delta_{i}\right) \\
& +\sum_{j} b_{j l} \prod_{i}\left(1+\epsilon_{j l i}^{b} \delta_{i}\right) \tag{2}
\end{align*}
$$

for luminosity $L$, Standard Model cross sections $\sigma_{l}$ (including efficiencies and acceptances), and expected backgrounds $b_{j l}$. Background estimates $b_{j l}$ may come either from Monte Carlo simulations or from control regions in which the expected number of events, $\bar{n}_{j l}$, is proportional to the expected background, via $b_{j l}=\alpha_{j l} \bar{n}_{j l}$. Given the number of observed events in the signal region $N_{l}^{\text {obs }}$, the likelihood function can be written as:
$\mathcal{L}_{l}=\operatorname{Pois}\left(N_{l}^{\mathrm{obs}} \mid N_{l}^{\mathrm{exp}}\right) \prod_{j_{l}} \operatorname{Pois}\left(n_{j l} \mid \bar{n}_{j l}\right) \prod_{i} G\left(m_{i} \mid \delta_{i}, 1\right)$,
where $n_{j l}$ are the observed numbers of background events in the control regions and $\operatorname{Pois}(x \mid y)$ is the Poisson probability of observing $x$ events given an expectation $y$.

The combined likelihood is given by the product of the individual likelihoods for each channel:
$\mathcal{L}=\prod_{l} \mathcal{L}_{l}$,
where $l$ is implicitly an index over the individual histogram bins within the channels that used a binned distribution of a discriminating variable.

The profile likelihood ratio
$\tilde{\lambda}(\mu)= \begin{cases}\frac{\mathcal{L}(\mu, \hat{\hat{\theta}}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\hat{\theta}})}, & \hat{\mu} \geq 0, \\ \frac{\mathcal{L}(\mu, \hat{\hat{\theta}}(\mu))}{\mathcal{L}(0, \hat{\theta}(0))}, & \hat{\mu}<0,\end{cases}$
is computed by maximising the likelihood function twice: in the numerator $\mu$, the ratio of the hypothesised cross section to the expected Standard Model cross section, is restricted
to a particular value and in the denominator $\mu$ is allowed to float. The set of all nuisance parameters $\delta_{i}$ and $\bar{n}_{j l}$ is denoted $\theta$. The maximum likelihood estimates of $\mu$ and $\theta$ are denoted $\hat{\mu}$ and $\hat{\theta}$, while $\hat{\hat{\theta}}(\mu)$ denotes the conditional maximum likelihood estimate of all nuisance parameters with $\mu$ fixed. In this analysis the range of $\mu$ is restricted to the physically meaningful regime, i.e. it is not allowed to be negative. The test statistic $\tilde{q}_{\mu}$ is defined to be

$$
\begin{align*}
\tilde{q}_{\mu} & = \begin{cases}-2 \ln \tilde{\lambda}(\mu), & \hat{\mu} \leq \mu \\
0, & \hat{\mu}>\mu\end{cases} \\
& = \begin{cases}-2 \ln \frac{\mathcal{L}(\mu, \hat{\hat{\theta}}(\mu))}{\mathcal{L}(0, \hat{\theta}(0))}, & \hat{\mu}<0 \\
-2 \ln \frac{\mathcal{L}(\mu, \hat{\hat{\theta}}(\mu))}{\mathcal{L}(\hat{\mu}, \hat{\theta})}, & 0 \leq \hat{\mu} \leq \mu \\
0, & \hat{\mu}>\mu\end{cases} \tag{4}
\end{align*}
$$

Monte Carlo pseudo-experiments are generated to construct the probability density function $f\left(\tilde{q}_{\mu} \mid \mu, \hat{\hat{\theta}}(\mu)\right)$ under an assumed signal strength $\mu$, giving a $p$-value
$p_{\mu}=\int_{\tilde{q}_{\mu, \mathrm{obs}}}^{\infty} f\left(\tilde{q}_{\mu} \mid \mu, \hat{\hat{\theta}}(\mu)\right) \mathrm{d} \tilde{q}_{\mu}$.
To find the upper limit on $\mu$ at $95 \%$ confidence level, $\mu_{\text {up }}$, $\mu$ is varied to find $p_{\mu_{\text {up }}}=5 \%$. Similarly, background-only Monte Carlo pseudo-experiments are used to find the median $\mu_{\text {med }}$ along with the $\pm 1 \sigma$ and $+2 \sigma$ bands expected in the absence of a signal. The procedure so far can be referred to as a $\mathrm{CL}_{s b}$ limit. To protect against excluding the (signal) null hypothesis in cases of downward fluctuations of the background, the observed limit is not allowed to fluctuate below the $-1 \sigma$ expected limit. This is equivalent to restricting the interval to cases in which the statistical power of the test of $\mu$ against the alternative $\mu=0$ is at least $16 \%$. This is referred to as a Power Constrained Limit. If the observed limit fluctuates below the $16 \%$ power, the quoted limit is $\mu_{\text {med }}-1 \sigma$.

## 8 Systematic uncertainties in the combination

The systematic uncertainty related to the luminosity is $\pm 3.4 \%$ and is fully correlated among all channels. It affects background estimates that are normalised to their theoretical cross sections; for most channels this is only true for backgrounds that are known to be small. In the $H \rightarrow Z Z \rightarrow \ell \ell \nu v$ and $H \rightarrow Z Z \rightarrow \ell \ell q q$ channels major backgrounds are normalised to their theoretical cross sections, but in the latter case this is only done after comparing with control regions.

Sources of systematic uncertainty related to the event reconstruction are correlated between all the Higgs boson search channels. The uncertainty on the efficiency to reconstruct electrons varies between $2.5 \%$ (central high- $p_{\text {T }}$ elec-
trons) and $16 \%$ ( $p_{\mathrm{T}}$ near 15 GeV , the lowest value used here) but it is assumed to be completely correlated. For muons the efficiency uncertainty ranges between $0.4 \%$ and $2 \%$. The jet systematic errors are typically larger for the channels where jets are explicitly required. They are dominated by the jet energy scale as the resolution effects tend to partially cancel and the $E_{\mathrm{T}}^{\text {miss }}$ uncertainties are largely by-products of the uncertainties already discussed.

The effect on the signal yield in each channel of the major sources of systematic uncertainty is summarised in Table 7. Uncertainties are treated as either uncorrelated or $100 \%$ correlated among channels. The largest uncorrelated errors are photon isolation in $H \rightarrow \gamma \gamma$ and jet rates in $H \rightarrow W W^{(*)} \rightarrow$ $\ell \nu \ell \nu$; the latter is in principle correlated with the $H \rightarrow$ $W W \rightarrow \ell \nu q q$ channel but these channels are never used in the same mass region. Most backgrounds have been estimated by means of independent control samples; these estimates are assumed to be uncorrelated between the channels.

Systematic uncertainties on the signal shape are accounted for in the $H \rightarrow \gamma \gamma, H \rightarrow Z Z \rightarrow \ell \ell q q$ and $H \rightarrow$ $Z Z \rightarrow \ell \ell \nu \nu$ channels by considering three possible distributions and interpolating between them. Small signal shape systematic uncertainties in the $H \rightarrow Z^{(*)} \rightarrow \ell \ell \ell \ell$ and $H \rightarrow W W \rightarrow \ell \nu q q$ channels are neglected. For $m_{H} \geq$ 200 GeV the correlations in the shape systematics are taken into account and are treated as correlated with the signal normalisation uncertainties.

The width of the Higgs boson signal at high mass is taken from the PYTHIA Monte Carlo [53]. This underestimates the width and the accepted cross section is conservatively scaled down by the ratio of the widths given in Ref. [69], which reached a maximum of $8 \%$ at 600 GeV , in all plots showing a ratio to the Standard Model.

The systematic uncertainty coming from the total theoretical Higgs boson cross section is not included in the combination and is shown separately in the figures as an uncertainty on the predicted cross section.

## 9 Combination

Each Higgs boson search channel is only sensitive for a range of Higgs boson masses. The ranges in which the various channels have been analysed are detailed in Table 8.

Table 8 The Higgs boson mass regions in which individual search channels have been analysed

| Mode | Mass range, GeV |
| :--- | :--- |
| $H \rightarrow \gamma \gamma$ | $110-140$ |
| $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ | $120-200$ |
| $H \rightarrow W W \rightarrow \ell \nu q q$ | $220-600$ |
| $H \rightarrow Z Z^{(*)} \rightarrow \ell \ell \ell$ | $120-600$ |
| $H \rightarrow Z Z \rightarrow \ell \ell \nu$ | $200-600$ |
| $H \rightarrow Z Z \rightarrow \ell \ell q q$ | $200-600$ |



Fig. 8 The expected and observed cross section limits, normalized to the Standard Model cross section, as a function of the Higgs boson mass for the individual search channels. The visually most apparent difference between expected and observed is in the $H \rightarrow W W \rightarrow \ell \nu q q$ channel, which has a deficit approaching one sigma both at 320 GeV and 480 GeV . These results use the profile likelihood method with a
power constraint (PCL). The limits are calculated at the masses marked with symbols. The lines between the points are to guide the eye. The grey horizontal bands show the uncertainty on the Standard Model cross section prediction, with the inner region highlighting the contribution of QCD scale uncertainties

In the $H \rightarrow \gamma \gamma, H \rightarrow Z Z \rightarrow \ell \ell \nu \nu$ and $H \rightarrow Z Z \rightarrow \ell \ell q q$ channels, the final result is extracted from a fit of signal plus background contributions to the observed Higgs boson candidate mass distributions. In all other channels, limits are extracted from a comparison of the numbers of observed events in one or more signal regions to the numbers of estimated background events.

The individual channels are shown in Fig. 8 in terms of the observed and the expected upper limits on $\sigma / \sigma_{\mathrm{S} M}$ at the $95 \%$ confidence level. The step with which the limit is extracted, $5-10 \mathrm{GeV}$, does not match the $H \rightarrow \gamma \gamma$ resolution which has a full-width at half maximum of 4.4 GeV . However, it was established in Ref. [7] that no important fluctuations are missed.

The search channels are grouped by the primary Higgs boson decay mode searched for, $\gamma \gamma, W W$ or $Z Z$, and the limit on each mode is extracted in terms of the cross section for the process intended. Some channels have a contribution from signal modes other then the intended one. This is only significant for the $H \rightarrow Z Z \rightarrow \ell \ell \nu v$ search, as discussed in Sect. 6.3, and implies that the $Z Z$ limit assumes the Standard Model ratio between $H$ to $Z Z$ and $H$ to $W W$ decays. In addition, the $W W$ search requires zero or one jet and is essentially designed for a spin-zero object produced largely via gluon fusion. The upper limits at $95 \%$ confidence level observed and expected in the absence of a signal are compared with the cross section expected for a Standard Model Higgs boson in Fig. 9.

Fig. 9 The expected and observed $95 \%$ PCL limits on the total cross section of a particle produced like the Standard Model Higgs boson and decaying with the width predicted by PYTHIA[53] to pairs of bosons: $\gamma \gamma, W W$ or $Z Z$. The limits are calculated at the masses marked with symbols. The lines between the points are to guide the eye. The coloured bands show the cross section predictions and their uncertainties, with the inner region highlighting the contribution of QCD scale uncertainties

Fig. 10 The expected and observed upper limits on the total cross section divided by the expected Standard Model Higgs boson cross section. This is a $95 \%$ PCL limit. The green and yellow bands indicate the range in which the limit is expected to lie in the absence of a signal. The fine dotted line marks the results obtained using $\mathrm{CL}_{s b}$, and the application of the power constraint gives the solid line. The limits are calculated at the masses marked with symbols and the lines between the points are to guide the eye



Table 9 The signal cross sections, in multiples of the Standard Model cross section, that are excluded, and expected to be excluded, at $95 \% \mathrm{CL}$. The expected variation at $\pm 1 \sigma$ is also given for the PCL limits. The bold numbers show the limit which should be used; for mass of 500 and 520 GeV the power constraint is applied. The likelihood ratio of signal plus background to background is also shown, as is the $p$-value (modified to go between 0 and 1) for $\mu=0$, which can be used to estimate the discovery significance

Fig. 11 Same as Fig. 10, except that limits calculated using the $\mathrm{CL}_{s}$ procedure are added. As expected, when the observed limits fluctuate up, both methods converge, but downward fluctuations are less pronounced with $\mathrm{CL}_{s}$ due to its larger over-coverage. The fine dotted line marks the results obtained using $\mathrm{CL}_{s b}$, and the application of the power constraint gives the solid line. The limits are calculated at the masses marked with symbols. The lines between the points are to guide the eye. The regions excluded by the combined LEP experiments [4] and the Tevatron experiments [6] are indicated

| $m_{H}(\mathrm{GeV})$ | PCL limits |  |  |  | $\mathrm{CL}_{s}$ limits |  | $-2 \ln \frac{\mathcal{L}(1, \hat{\hat{\theta}})}{\mathcal{L}(0, \hat{\theta})}$ | $p$-values$p_{\mu=0}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Obs. | $-1 \sigma$ | Median | $+1 \sigma$ | Obs. | Median |  |  |
| 110 | 18.7 | 6.9 | 21.5 | 38.2 | 28.1 | 29.6 | 0.1 | 0.58 |
| 115 | 42.4 | 7.8 | 20.9 | 34.7 | 43.5 | 25.3 | -0.3 | 0.07 |
| 120 | 18.2 | 4.3 | 11.4 | 19.9 | 19.7 | 15.4 | -0.3 | 0.22 |
| 130 | 10.0 | 2.5 | 6.4 | 10.9 | 11.0 | 8.5 | -0.6 | 0.23 |
| 140 | 5.0 | 1.7 | 4.3 | 7.6 | 6.1 | 5.9 | 0.0 | 0.41 |
| 150 | 2.5 | 1.3 | 3.2 | 5.5 | 4.0 | 4.4 | 1.0 | 0.65 |
| 160 | 1.6 | 0.7 | 2.3 | 3.9 | 2.8 | 3.1 | 1.6 | 0.68 |
| 170 | 3.4 | 0.8 | 2.4 | 3.9 | 3.8 | 3.1 | -0.4 | 0.27 |
| 180 | 5.3 | 1.0 | 3.0 | 5.4 | 5.6 | 4.2 | -0.9 | 0.18 |
| 190 | 8.8 | 1.9 | 4.8 | 7.8 | 9.2 | 6.3 | -1.1 | 0.11 |
| 200 | 9.7 | 2.1 | 5.4 | 9.5 | 9.9 | 7.5 | $-1.1$ | 0.15 |
| 220 | 15.9 | 2.9 | 10.0 | 15.4 | 17.1 | 12.9 | 0.0 | 0.13 |
| 240 | 8.3 | 2.5 | 9.1 | 14.5 | 11.2 | 11.9 | 0.3 | 0.57 |
| 260 | 7.4 | 2.9 | 7.7 | 12.6 | 10.8 | 10.9 | 0.4 | 0.56 |
| 280 | 10.0 | 2.5 | 7.3 | 13.9 | 11.5 | 10.2 | 0.2 | 0.31 |
| 300 | 9.5 | 1.9 | 7.2 | 13.2 | 11.4 | 10.1 | 0.2 | 0.32 |
| 320 | 7.1 | 2.5 | 6.2 | 12.1 | 9.8 | 9.5 | 0.4 | 0.40 |
| 340 | 9.0 | 2.8 | 6.5 | 11.9 | 9.9 | 9.6 | 0.4 | 0.28 |
| 360 | 5.5 | 2.5 | 7.7 | 12.5 | 8.5 | 9.5 | 0.4 | 0.63 |
| 380 | 5.6 | 2.2 | 7.3 | 12.9 | 8.6 | 9.5 | 0.4 | 0.53 |
| 400 | 7.5 | 2.4 | 7.8 | 13.6 | 9.4 | 9.6 | 0.1 | 0.49 |
| 420 | 8.0 | 2.9 | 8.4 | 14.7 | 10.4 | 10.4 | 0.2 | 0.46 |
| 440 | 9.8 | 3.5 | 9.9 | 15.8 | 11.7 | 11.8 | 0.1 | 0.46 |
| 460 | 6.3 | 3.1 | 8.7 | 18.1 | 10.1 | 12.3 | 0.4 | 0.64 |
| 480 | 5.6 | 3.7 | 10.1 | 17.7 | 10.4 | 13.4 | 0.4 | 0.80 |
| 500 | 3.1 | 5.0 | 9.9 | 19.3 | 11.8 | 15.9 | 0.5 | 0.89 |
| 520 | 4.8 | 5.3 | 14.1 | 23.1 | 13.9 | 18.5 | 0.4 | 0.86 |
| 540 | 6.3 | 5.6 | 16.7 | 26.0 | 16.8 | 21.3 | 0.4 | 0.82 |
| 560 | 8.0 | 6.6 | 16.9 | 33.5 | 19.3 | 23.7 | 0.3 | 0.80 |
| 580 | 19.7 | 10.2 | 22.2 | 37.9 | 27.5 | 28.8 | 0.1 | 0.56 |
| 600 | 26.1 | 10.6 | 24.0 | 49.2 | 34.4 | 33.9 | 0.1 | 0.45 |



Fig. 12 Same as Fig. 10, but comparing the excluded cross section to the expected one when a fourth generation of high mass quarks and leptons with Standard Model-like couplings to the Higgs boson are included in the cross section calculations. The arrows indicate the regions excluded by the CMS experiment [12] and the Tevatron experiments [70]. The point set at 500 GeV is at the limit allowed by the power constraint. The limits are calculated at the masses marked with symbols. The lines between the points are to guide the eye


Table 10 The signal cross sections, in multiples of the high mass fourth generation model [50] cross section, that are excluded, and expected to be excluded, in the absence of signal, at $95 \%$ CL

| $m_{H}(\mathrm{GeV})$ | PCL limits |  |  | $\mathrm{CL}_{s}$ limits |  | $m_{H}(\mathrm{GeV})$ | PCL limits |  |  | $\mathrm{CL}_{s}$ limits |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Obs. | $-1 \sigma$ | Median | Median | Obs. |  | Obs. | $-1 \sigma$ | Median | Median | Obs. |
| 110 | 17.1 | 7.8 | 19.6 | 25.2 | 23.9 | 320 | 1.3 | 0.4 | 1.1 | 1.7 | 1.8 |
| 115 | 35.8 | 6.7 | 17.0 | 22.4 | 36.6 | 340 | 1.7 | 0.5 | 1.2 | 1.9 | 1.9 |
| 120 | 4.3 | 1.2 | 2.8 | 3.8 | 4.8 | 360 | 1.3 | 0.6 | 1.7 | 2.0 | 1.9 |
| 130 | 2.0 | 0.5 | 1.2 | 1.6 | 2.1 | 380 | 1.5 | 0.7 | 1.8 | 2.1 | 2.0 |
| 140 | 0.9 | 0.2 | 0.7 | 0.9 | 1.0 | 400 | 2.0 | 0.8 | 1.9 | 2.2 | 2.3 |
| 150 | 0.4 | 0.2 | 0.4 | 0.6 | 0.5 | 420 | 2.1 | 0.9 | 2.0 | 2.6 | 2.5 |
| 160 | 0.2 | 0.1 | 0.3 | 0.4 | 0.3 | 440 | 2.6 | 1.1 | 2.2 | 2.8 | 3.0 |
| 170 | 0.4 | 0.1 | 0.3 | 0.4 | 0.4 | 460 | 1.6 | 1.2 | 2.4 | 3.0 | 2.6 |
| 180 | 0.6 | 0.1 | 0.4 | 0.5 | 0.7 | 480 | 1.5 | 1.0 | 2.5 | 3.3 | 2.9 |
| 190 | 1.1 | 0.2 | 0.6 | 0.8 | 1.1 | 500 | 0.8 | 1.4 | 3.0 | 3.5 | 3.0 |
| 200 | 1.2 | 0.3 | 0.7 | 1.0 | 1.3 | 520 | 1.3 | 0.9 | 3.0 | 4.1 | 3.6 |
| 220 | 2.3 | 0.5 | 1.2 | 1.8 | 2.4 | 540 | 1.7 | 1.5 | 3.3 | 4.3 | 3.8 |
| 240 | 1.2 | 0.4 | 1.1 | 1.7 | 1.7 | 560 | 1.8 | 1.8 | 4.3 | 5.4 | 4.6 |
| 260 | 1.1 | 0.4 | 1.1 | 1.6 | 1.6 | 580 | 4.8 | 1.8 | 4.6 | 6.0 | 6.3 |
| 280 | 1.6 | 0.4 | 1.1 | 1.6 | 1.9 | 600 | 6.4 | 2.5 | 5.5 | 7.4 | 7.8 |
| 300 | 1.5 | 0.4 | 1.1 | 1.6 | 1.9 |  |  |  |  |  |  |

The combination of all channels is tested and the $p_{\mu=0}$ in these fits varies between $7 \%$ and $89 \%$, which does not suggest the presence of a signal. The combination of all channels is shown in Fig. 10 in terms of the observed and the expected upper limit at the $95 \%$ confidence level. The statistical accuracy of the toy Monte Carlo used to extract the limits is about $5 \%$ on the observed limits and $7 \%$ on the expected ones, with somewhat larger variation on the edges of the one and two $\sigma$ bands.

The excluded signal strength as a function of $m_{H}$ is summarised in Table 9, using the PCL method. The results are also calculated using the $\mathrm{CL}_{s}$ method for comparison pur-
poses: the extracted limits from both procedures are shown in Fig. 11. Also given is the profile likelihood ratio of a Standard Model Higgs boson to background only and the consistency of the data with the background-only hypothesis,
$p_{\mu=0}$.
The results have been interpreted in terms of the heavy mass fourth generation model introduced in Sect. 3. This involves rescaling the gluon fusion component of the production cross section and the Higgs boson decay branching ratios. The limits are shown in Fig. 12. This model is excluded for Higgs boson masses between 140 GeV and 185 GeV ,
while the region in which exclusion might be expected is between 136 GeV and 208 GeV .

The excluded cross section ratios are summarised in Table 10 .

## 10 Conclusions

The ATLAS search for the Standard Model Higgs boson in the mass range from 110 GeV to 600 GeV in 35 to $40 \mathrm{pb}^{-1}$ of data recorded in 2010 has been presented. With this luminosity there is not sufficient sensitivity to exclude the Standard Model Higgs boson, nor is there any evidence of an excess of events over the predicted background rates. However, these results give the most stringent constraints to date for Higgs boson masses above 250 GeV and are close to the Tevatron limits [6] at intermediate masses.

An extension of the Standard Model, assuming the Higgs mechanism and adding a fourth generation of heavy quarks and leptons, is excluded for Higgs boson masses between 140 and 185 GeV .

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# Search for charged Higgs bosons decaying via $H^{ \pm} \rightarrow \tau \nu$ in $t \bar{t}$ events using $p p$ collision data at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

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Abstract: The results of a search for charged Higgs bosons are presented. The analysis is based on $4.6 \mathrm{fb}^{-1}$ of proton-proton collision data at $\sqrt{s}=7 \mathrm{TeV}$ collected by the ATLAS experiment at the Large Hadron Collider, using top quark pair events with a $\tau$ lepton in the final state. The data are consistent with the expected background from Standard Model processes. Assuming that the branching ratio of the charged Higgs boson to a $\tau$ lepton and a neutrino is $100 \%$, this leads to upper limits on the branching ratio of top quark decays to a $b$ quark and a charged Higgs boson between $5 \%$ and $1 \%$ for charged Higgs boson masses ranging from 90 GeV to 160 GeV , respectively. In the context of the $m_{h}^{\max }$ scenario of the MSSM, $\tan \beta$ above 12-26, as well as between 1 and 2-6, can be excluded for charged Higgs boson masses between 90 GeV and 150 GeV .

Keywords: Hadron-Hadron Scattering

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## 1 Introduction

Charged Higgs bosons $\left(H^{+}, H^{-}\right)$are predicted by several non-minimal Higgs scenarios, such as Two Higgs Doublet Models (2HDM) [1] or models containing Higgs triplets [2-6]. As the Standard Model (SM) does not contain any elementary charged scalar particle, the observation of a charged Higgs boson ${ }^{1}$ would clearly indicate new physics beyond the SM. For instance, supersymmetric models predict the existence of charged Higgs bosons. In a type-II 2HDM, such as the Higgs sector of the Minimal Supersymmetric extension of the Standard Model (MSSM) [7-11], the main $H^{+}$production mode at the Large Hadron Collider (LHC) is through top quark decays $t \rightarrow b H^{+}$, for charged Higgs boson masses ( $m_{H^{+}}$) smaller than the top quark mass $\left(m_{\text {top }}\right)$. The dominant source of top quarks at the LHC is through $t \bar{t}$ production. The cross section for $H^{+}$production from single top quark events is much smaller and is not considered here. For $\tan \beta>2$, where $\tan \beta$ is the ratio of the vacuum expectation values of the two Higgs doublets, the charged Higgs boson decay via $H^{+} \rightarrow \tau \nu$ is dominant and remains sizeable for $1<\tan \beta<2$ [12]. In this paper, $\mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)=100 \%$ is assumed, unless otherwise specified. Under this assumption, the combined LEP lower limit for the charged Higgs boson mass is about 90 GeV [13]. The Tevatron experiments placed upper limits on $\mathcal{B}\left(t \rightarrow b H^{+}\right)$in the $15-20 \%$ range for $m_{\mathrm{H}^{+}}<m_{\text {top }}[14,15]$.

This paper describes a search for charged Higgs bosons with masses in the range 90160 GeV , using $t \bar{t}$ events with a leptonically or hadronically decaying $\tau$ lepton in the final state, i.e. with the topology shown in figure 1. Charged Higgs bosons are searched for in a model-independent way, hence exclusion limits are given in terms of $\mathcal{B}\left(t \rightarrow b H^{+}\right)$, as well as in the $m_{h}^{\max }$ scenario [16] of the MSSM. The results are based on $4.6 \mathrm{fb}^{-1}$ of data from $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$, collected in 2011 with the ATLAS experiment [17] at the LHC. Three final states, which are expected to yield the highest sensitivity, are analysed:

- lepton+jets: $t \bar{t} \rightarrow b \bar{b} W H^{+} \rightarrow b \bar{b}\left(q \bar{q}^{\prime}\right)\left(\tau_{\text {lep }} \nu\right)$, i.e. $W$ decays hadronically and $\tau$ decays into an electron or a muon, with two neutrinos;
- $\tau+$ lepton: $t \bar{t} \rightarrow b \bar{b} W H^{+} \rightarrow b \bar{b}(l \nu)\left(\tau_{\text {had }} \nu\right)$, i.e. $W$ decays leptonically (with $l=e, \mu$ ) and $\tau$ decays hadronically;
- $\tau+$ jets: $t \bar{t} \rightarrow b \bar{b} W H^{+} \rightarrow b \bar{b}\left(q \bar{q}^{\prime}\right)\left(\tau_{\text {had }} \nu\right)$, i.e. both $W$ and $\tau$ decay hadronically.

In section 2, the data and simulated samples used in this analysis are described. In section 3, the reconstruction of physics objects in ATLAS is discussed. Sections 4-6 present results obtained in the lepton + jets, $\tau+$ lepton and $\tau+$ jets channels, respectively. Systematic uncertainties are discussed in section 7 , before exclusion limits in terms of $\mathcal{B}\left(t \rightarrow b H^{+}\right)$ and $\tan \beta$ are presented in section 8 . Finally, a summary is given in section 9.

[^46]

Figure 1. Example of a leading-order Feynman diagram for the production of $t \bar{t}$ events arising from gluon fusion, where a top quark decays to a charged Higgs boson, followed by the decay $H^{+} \rightarrow \tau \nu$.

## 2 Data and simulated events

The ATLAS detector [17] consists of an inner tracking detector with a coverage in pseudorapidity ${ }^{2}$ up to $|\eta|=2.5$, surrounded by a thin 2 T superconducting solenoid, a calorimeter system extending up to $|\eta|=4.9$ for the detection of electrons, photons and hadronic jets, and a large muon spectrometer extending up to $|\eta|=2.7$ that measures the deflection of muon tracks in the field of three superconducting toroid magnets. A three-level trigger system is used. The first level trigger is implemented in hardware, using a subset of detector information to reduce the event rate to a design value of at most 75 kHz . This is followed by two software-based trigger levels, which together reduce the event rate to about 300 Hz .

Only data taken with all ATLAS sub-systems operational are used; this results in an integrated luminosity of $4.6 \mathrm{fb}^{-1}$ for the 2011 data-taking period. The integrated luminosity has an uncertainty of $3.9 \%$, measured as described in refs. [18, 19] and based on the whole 2011 dataset. Following basic data quality checks, further event cleaning is performed by demanding that no jet is consistent with having originated from instrumental effects, such as large noise signals in one or several channels of the hadronic end-cap calorimeter, coherent noise in the electromagnetic calorimeter, or non-collision backgrounds. In addition, events are discarded if the reconstructed vertex with the largest sum of squared track momenta has fewer than five associated tracks with transverse momenta $p_{\mathrm{T}}>400 \mathrm{MeV}$.

The background processes that enter this search include the SM pair production of top quarks $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$, as well as the production of single top quark, $W+$ jets, $Z / \gamma^{*}+$ jets, diboson and multi-jet events. Data-driven methods are used in order to estimate the multijet background, as well as the backgrounds with intrinsic missing transverse momentum where electrons or jets are misidentified as hadronically decaying $\tau$ leptons. The modelling of SM $t \bar{t}$ and single top quark events is performed with MC@NLO [20], except for the

[^47]| Process | Generator | Cross section [pb] |  |
| :--- | :--- | :--- | :--- |
| SM $t \bar{t}$ with at least one lepton $\ell=e, \mu, \tau$ | MC@NLO $[20]$ | 91 | $[26]$ |
| Single top quark $t$-channel (with $\ell$ ) | AcerMC | $[21]$ | 21 |
| Single top quark $s$-channel (with $\ell)$ | MC@NLO $[20]$ | 1.5 | $[27]$ |
| Single top quark $W t$-channel (inclusive) | MC@NLO $[20]$ | 16 | $[29]$ |
| $W \rightarrow \ell \nu$ | ALPGEN $[31]$ | $3.1 \times 10^{4}$ | $[33]$ |
| $Z / \gamma^{*} \rightarrow \ell$ with $m(\ell \ell)>10 \mathrm{GeV}$ | ALPGEN $[31]$ | $1.5 \times 10^{4}$ | $[34]$ |
| $W W$ | HERWIG $[23]$ | 17 | $[35]$ |
| $Z Z$ | HERWIG $[23]$ | 1.3 | $[35]$ |
| $W Z$ | HERWIG | $[23]$ | 5.5 |
| $H^{+}$signal with $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$ | PYTHIA | $[25]$ | 16 |

Table 1. Cross sections for the simulated processes and generators used to model them.
$t$-channel single top quark production where AcerMC [21] is used. The top quark mass is set to 172.5 GeV and the set of parton distribution functions used is CT10 [22]. For the events generated with MC@NLO, the parton shower, hadronisation and underlying event are added using HERWIG [23] and JIMMY [24]. PYTHIA [25] is instead used for events generated with AcerMC. Inclusive cross sections are taken from the approximate next-to-next-to-leading-order (NNLO) predictions for $t \bar{t}$ production [26], for single top quark production in the $t$-channel and $s$-channel [27, 28], as well as for $W t$ production [29]. Overlaps between $W t$ and SM $t \bar{t}$ final states are removed [30]. Single vector boson ( $W$ and $Z / \gamma^{*}$ ) production is simulated with ALPGEN [31] interfaced to HERWIG and JIMMY, using CTEQ6.1 [32] parton distribution functions. The additional partons produced in the matrix element part of the event generation can be light partons or heavy quarks. In the latter case, dedicated samples with matrix elements for the production of massive $b \bar{b}$ or $c \bar{c}$ pairs are used. Diboson events ( $W W, W Z$ and $Z Z$ ) are generated using HERWIG. The cross sections are normalised to NNLO predictions for $W$ and $Z / \gamma^{*}$ production [33, 34] and to next-to-leading-order (NLO) predictions for diboson production [35].

The SM background samples are summarised in table 1. In addition, three types of signal samples are produced with PYTHIA for $90 \mathrm{GeV}<m_{H^{+}}<160 \mathrm{GeV}: t \bar{t} \rightarrow b \bar{b} H^{+} W^{-}$, $t \bar{t} \rightarrow b \bar{b} H^{-} W^{+}$and $t \bar{t} \rightarrow b \bar{b} H^{+} H^{-}$, where the charged Higgs bosons decay as $H^{+} \rightarrow \tau \nu$. The cross section for each of these three processes depends only on the total $t \bar{t}$ production cross section ( 167 pb ) and the branching ratio $\mathcal{B}\left(t \rightarrow b H^{+}\right)$. TAUOLA [36] is used for $\tau$ decays, and PHOTOS [37] is used for photon radiation from charged leptons.

The event generators are tuned in order to describe the ATLAS data. The parameter sets AUET2 [38] and AUET2B [39] are used for events for which hadronisation is simulated using HERWIG/JIMMY and PYTHIA, respectively. To take into account the presence of multiple interactions (around nine, on average) occurring in the same and neighbouring
bunch crossings (referred to as pile-up), simulated minimum bias events are added to the hard process in each generated event. Prior to the analysis, simulated events are reweighted in order to match the distribution of the average number of pile-up interactions in the data. All generated events are propagated through a detailed GEANT4 simulation [40, 41] of the ATLAS detector and are reconstructed with the same algorithms as the data.

## 3 Physics object reconstruction

### 3.1 Electrons

Electrons are reconstructed by matching clustered energy deposits in the electromagnetic calorimeter to tracks reconstructed in the inner detector. The electron candidates are required to meet quality requirements based on the expected shower shape [42], to have a transverse energy $E_{\mathrm{T}}>20 \mathrm{GeV}$ and to be in the fiducial volume of the detector, $|\eta|<2.47$ (the transition region between the barrel and end-cap calorimeters, $1.37<|\eta|<1.52$, is excluded). Additionally, $E_{\mathrm{T}}$ and $\eta$-dependent calorimeter (tracking) isolation requirements are imposed in a cone with a radius ${ }^{3} \Delta R=0.2(0.3)$ around the electron position, excluding the electron object itself, with an efficiency of about $90 \%$ for true isolated electrons.

### 3.2 Muons

Muon candidates are required to contain matching inner detector and muon spectrometer tracks [43], as well as to have $p_{\mathrm{T}}>15 \mathrm{GeV}$ and $|\eta|<2.5$. Only isolated muons are accepted by requiring that the transverse energy deposited in the calorimeters (the transverse momentum of the inner detector tracks) in a cone of radius $\Delta R=0.2(0.3)$ around the muon amounts to less than $4 \mathrm{GeV}(2.5 \mathrm{GeV})$. The energy and momentum of the muon are excluded from the cone when applying these isolation requirements.

### 3.3 Jets

Jets are reconstructed using the anti- $k_{t}$ algorithm [44, 45] with a size parameter value of $R=0.4$. The jet finder uses reconstructed three-dimensional, noise-suppressed clusters of calorimeter cells [46]. Jets are calibrated to the hadronic energy scale with correction factors based on simulation [47, 48]. A method that allows for the identification and selection of jets originating from the hard-scatter interaction through the use of tracking and vertexing information is used [49]. This is referred to as the "Jet Vertex Fraction" (JVF), defined as the fraction of the total momentum of the charged particle tracks associated to the jet which belongs to tracks that are also compatible with the primary vertex. By convention, jets with no associated tracks are assigned a JVF value of -1 in order to keep a high efficiency for jets at large values of $\eta$, outside the range of the inner tracking detectors. The jet selection based on this discriminant is shown to be insensitive to pile-up. A requirement of $|J V F|>0.75$ is placed on all jets during event selection. In order to identify the jets initiated by $b$ quarks, an algorithm is used that combines impact-parameter information

[^48]with the explicit determination of a secondary vertex [50]. A working point is chosen that corresponds to an average efficiency of about $70 \%$ for $b$ jets with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $t \bar{t}$ events and a light-quark jet rejection factor of about 130 . Since the $b$-tagger relies on the inner tracking detectors, the acceptance region for jets is restricted to $|\eta|<2.4$.

## $3.4 \quad \tau$ jets

In order to reconstruct hadronically decaying $\tau$ leptons, anti- $k_{t}$ jets with either one or three associated tracks reconstructed in the inner detector and depositing $E_{\mathrm{T}}>10 \mathrm{GeV}$ in the calorimeter are considered as $\tau$ candidates [51]. Dedicated algorithms are used in order to reject electrons and muons. Hadronic $\tau$ decays are identified using a likelihood criterion designed to discriminate against quark- and gluon-initiated jets by using the shower shape and tracking variables as inputs. A working point with an efficiency of about $30 \%$ for hadronically decaying $\tau$ leptons with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $Z \rightarrow \tau \tau$ events is chosen, leading to a rejection factor of about $100-1000$ for jets. The rejection factor depends on the $p_{\mathrm{T}}$ and $\eta$ of the candidate and the number of associated tracks. The $\tau$ candidates are further required to have a visible transverse momentum of at least 20 GeV and to be within $|\eta|<2.3$. The selected $\tau$ candidates are henceforth referred to as " $\tau$ jets".

### 3.5 Removal of geometric overlaps between objects

When candidates selected using the criteria above overlap geometrically, the following procedures are applied, in this order: muon candidates are rejected if they are found within $\Delta R<0.4$ of any jet with $p_{\mathrm{T}}>25 \mathrm{GeV} ;$ a $\tau$ jet is rejected if found within $\Delta R<0.2$ of a selected muon or electron; jets are removed if they are within $\Delta R<0.2$ of a selected $\tau$ object or electron.

### 3.6 Missing transverse momentum

The missing transverse momentum and its magnitude $E_{\mathrm{T}}^{\text {miss }}$ [52] are reconstructed from three-dimensional, noise-suppressed clusters of cells in the calorimeter and from muon tracks reconstructed in the muon spectrometer and the inner tracking detectors. Clusters of calorimeter cells belonging to jets (including $\tau$ jets) with $p_{\mathrm{T}}>20 \mathrm{GeV}$ are calibrated to the hadronic energy scale. Calorimeter cells not associated with any object are also taken into account and they are calibrated at the electromagnetic energy scale. In order to deal appropriately with the energy deposited by muons in the calorimeters, the contributions of muons to $E_{\mathrm{T}}^{\text {miss }}$ are calculated differently for isolated and non-isolated muons.

## 4 Analysis of the lepton+jets channel

This analysis relies on the detection of lepton+jets decays of $t \bar{t}$ events, where the charged lepton $l$ (electron or muon) arises from $H^{+} \rightarrow \tau_{\text {lep }} \nu$, while the jets arise from a hadronically decaying $W$ boson, i.e. $t \bar{t} \rightarrow b \bar{b} W H^{+} \rightarrow b \bar{b}\left(q \bar{q}^{\prime}\right)\left(\tau_{\text {lep }} \nu\right)$.

### 4.1 Event selection

The lepton + jets analysis uses events passing a single-lepton trigger with an $E_{\mathrm{T}}$ threshold of $20-22 \mathrm{GeV}$ for electrons ${ }^{4}$ and a $p_{\mathrm{T}}$ threshold of 18 GeV for muons. These thresholds are low enough to guarantee that electrons and muons chosen for the analysis are in the plateau region of the trigger-efficiency curve. In addition, to select a sample of lepton+jets events enriched in $t \bar{t}$ candidates, the following requirements are applied:

- exactly one lepton having $E_{\mathrm{T}}>25 \mathrm{GeV}$ (electron) or $p_{\mathrm{T}}>20 \mathrm{GeV}$ (muon) and matched to the corresponding trigger object, with neither a second lepton nor a $\tau$ jet in the event;
- at least four jets having $p_{\mathrm{T}}>20 \mathrm{GeV}$, with exactly two of them being $b$-tagged;
- $E_{\mathrm{T}}^{\text {miss }}>40 \mathrm{GeV}$ and, in order to discriminate between $E_{\mathrm{T}}^{\text {miss }}$ arising from isolated neutrinos and from poorly reconstructed leptons, this requirement is tightened to $E_{\mathrm{T}}^{\text {miss }} \times\left|\sin \Delta \phi_{l, \text { miss }}\right|>20 \mathrm{GeV}$ if the azimuthal angle $\Delta \phi_{l \text {,miss }}$ between the lepton and $E_{\mathrm{T}}^{\mathrm{miss}}$ is smaller than $\pi / 6$.

Having selected a lepton + jets sample enriched in $t \bar{t}$ candidates, jets must be assigned correctly to the decay products of each $W$ boson (with a mass $m_{W}=80.4 \mathrm{GeV}$ ) and top quark. In particular, the hadronic side of the event is identified by selecting the combination of one $b$-tagged jet ( $b$ ) and two untagged jets $(j)$ that minimises:

$$
\begin{equation*}
\chi^{2}=\frac{\left(m_{j j b}-m_{\mathrm{top}}\right)^{2}}{\sigma_{\mathrm{top}}^{2}}+\frac{\left(m_{j j}-m_{W}\right)^{2}}{\sigma_{W}^{2}} \tag{4.1}
\end{equation*}
$$

where $\sigma_{\text {top }}=17 \mathrm{GeV}$ and $\sigma_{W}=10 \mathrm{GeV}$ are the widths of the reconstructed top quark and $W$ boson mass distributions, as measured in simulated $t \bar{t}$ events. Using information about the correctly identified combinations in the generated events, the jet assignment efficiency is found to be $72 \%$. Events with $\chi^{2}>5$ are rejected in order to select well-reconstructed hadronic top quark candidates.

### 4.2 Data-driven estimation of backgrounds with misidentified leptons

While the ATLAS lepton identification gives a very pure sample of candidates, there is a non-negligible contribution from non-isolated leptons arising from the semileptonic decay of hadrons containing $b$ or $c$ quarks, from the decay-in-flight of $\pi^{ \pm}$or $K$ mesons and, in the case of misidentified electron objects, from the reconstruction of $\pi^{0}$ mesons, photon conversions or shower fluctuations. All leptons coming from such mechanisms are referred to as misidentified leptons, as opposed to truly isolated leptons (e.g. from the prompt decay of $W$ or $Z$ bosons), which are referred to as real leptons. The data-driven estimation of the number of misidentified leptons passing the lepton selections of sections 3.1 and 3.2 is based on exploiting differences in the lepton identification between real and misidentified

[^49]electrons or muons. Two data samples are defined, which differ only in the lepton identification criteria. The tight sample contains mostly events with real leptons and uses the same lepton selection as in the analysis. The loose sample contains mostly events with misidentified leptons. This latter sample is obtained by loosening the isolation and identification requirements for the leptons. For loose electrons, the isolation requirements have an efficiency of about $98 \%$ for true isolated electrons, compared to $90 \%$ in the tight sample. For loose muons, the isolation requirement is removed. By construction, the tight sample is therefore a subset of the loose sample.

Let $N_{\mathrm{r}}^{\mathrm{L}}$ and $N_{\mathrm{m}}^{\mathrm{L}}\left(N_{\mathrm{r}}^{\mathrm{T}}\right.$ and $N_{\mathrm{m}}^{\mathrm{T}}$ ) be the number of events containing real and misidentified leptons, respectively, passing a loose (tight) selection. The numbers of events containing one loose or tight lepton are given by:

$$
\begin{align*}
& N^{\mathrm{L}}=N_{\mathrm{m}}^{\mathrm{L}}+N_{\mathrm{r}}^{\mathrm{L}},  \tag{4.2}\\
& N^{\mathrm{T}}=N_{\mathrm{m}}^{\mathrm{T}}+N_{\mathrm{r}}^{\mathrm{T}} . \tag{4.3}
\end{align*}
$$

Defining $p_{\mathrm{r}}$ and $p_{\mathrm{m}}$ as:

$$
\begin{equation*}
p_{\mathrm{r}}=\frac{N_{\mathrm{r}}^{\mathrm{T}}}{N_{\mathrm{r}}^{\mathrm{L}}} \quad \text { and } \quad p_{\mathrm{m}}=\frac{N_{\mathrm{m}}^{\mathrm{T}}}{N_{\mathrm{m}}^{\mathrm{L}}} \text {, } \tag{4.4}
\end{equation*}
$$

the number of misidentified leptons passing the tight selection $N_{\mathrm{m}}^{\mathrm{T}}$ can then be written as:

$$
\begin{equation*}
N_{\mathrm{m}}^{\mathrm{T}}=\frac{p_{\mathrm{m}}}{p_{\mathrm{r}}-p_{\mathrm{m}}}\left(p_{\mathrm{r}} N^{\mathrm{L}}-N^{\mathrm{T}}\right) \tag{4.5}
\end{equation*}
$$

The main ingredients of this data-driven method are thus the relative efficiencies $p_{\mathrm{r}}$ and $p_{\mathrm{m}}$ for a real or a misidentified lepton, respectively, to be detected as a tight lepton. The lepton identification efficiency $p_{\mathrm{r}}$ is measured using a tag-and-probe method on $Z \rightarrow l l$ data events with a dilepton invariant mass between 86 GeV and 96 GeV , where one lepton is required to fulfill tight selection criteria. The rate at which the other lepton passes the same tight selection criteria defines $p_{\mathrm{r}}$. The average values of the electron and muon identification efficiencies are $80 \%$ and $97 \%$, respectively. On the other hand, a control sample with misidentified leptons is selected by considering events in the data with exactly one lepton passing the loose criteria. In order to select events dominated by multi-jet production, $E_{\mathrm{T}}^{\text {miss }}$ is required to be between 5 GeV and 20 GeV . Residual true leptons contribute at a level below $10 \%$ and are subtracted from this sample using simulation. After this subtraction, the rate at which a loose lepton passes tight selection criteria defines the misidentification rate $p_{\mathrm{m}}$. The average values of the electron and muon misidentification probabilities are $18 \%$ and $29 \%$, respectively. In the final parameterisation of $p_{\mathrm{r}}$ and $p_{\mathrm{m}}$, dependencies on the pseudorapidity of the lepton, its distance $\Delta R$ to the nearest jet and the leading jet $p_{\mathrm{T}}$ are taken into account.

### 4.3 Reconstruction of discriminating variables after the selection cuts

The analysis uses two variables that discriminate between leptons produced in $\tau \rightarrow l_{l} \nu_{\tau}$ and leptons coming directly from $W$ boson decays. The first discriminating variable is the
invariant mass $m_{b l}$ of the $b$ jet and the charged lepton $l$ coming from the same top quark candidate, or more conveniently, $\cos \theta_{l}^{*}$ defined as:

$$
\begin{equation*}
\cos \theta_{l}^{*}=\frac{2 m_{b l}^{2}}{m_{\mathrm{top}}^{2}-m_{W}^{2}}-1 \simeq \frac{4 p^{b} \cdot p^{l}}{m_{\mathrm{top}}^{2}-m_{W}^{2}}-1 . \tag{4.6}
\end{equation*}
$$

Both $m_{b}^{2}$ and $m_{l}^{2}$ are neglected, hence $m_{b l}^{2} \simeq 2 p^{b} \cdot p^{l}$, where $p^{b}$ and $p^{l}$ are the four-momenta of the $b$ jet and of the charged lepton $l$, respectively. The presence of a charged Higgs boson in a leptonic top quark decay reduces the invariant product $p^{b} \cdot p^{l}$, when compared to $W$-mediated top quark decays, leading to $\cos \theta_{l}^{*}$ values closer to -1 .

The second discriminating variable is the transverse mass $m_{\mathrm{T}}^{H}$ [53], obtained by fulfilling the constraint $\left(p^{\text {miss }}+p^{l}+p^{b}\right)^{2}=m_{\text {top }}^{2}$ on the leptonic side of lepton + jets $t \bar{t}$ events. More than one neutrino accounts for the invisible four-momentum $p^{\text {miss }}$ and its transverse component $\overrightarrow{p_{\mathrm{T}}}{ }^{\text {miss }}$. By construction, $m_{\mathrm{T}}^{H}$ gives an event-by-event lower bound on the mass of the leptonically decaying charged ( $W$ or Higgs) boson produced in the top quark decay, and it can be written as:

$$
\begin{equation*}
\left(m_{\mathrm{T}}^{H}\right)^{2}=\left(\sqrt{m_{\mathrm{top}}^{2}+\left({\overrightarrow{p_{\mathrm{T}}}}^{l}+{\overrightarrow{p_{\mathrm{T}}}}^{b}+{\overrightarrow{p_{\mathrm{T}}}}^{\text {miss }}\right)^{2}}-p_{\mathrm{T}}^{b}\right)^{2}-\left({\overrightarrow{p_{\mathrm{T}}}}^{l}+{\overrightarrow{p_{\mathrm{T}}}}^{\text {miss }}\right)^{2} . \tag{4.7}
\end{equation*}
$$

The $\cos \theta_{l}^{*}$ distribution measured in the data is shown in figure 2a, superimposed on the predicted background, determined with a data-driven method for the multi-jet background and simulation for the other SM backgrounds. In the presence of a charged Higgs boson in the top quark decays, with a branching ratio $\mathcal{B}\left(t \rightarrow b H^{+}\right)$, the contribution of $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$events in the background is scaled according to this branching ratio. A control region enriched in $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$events is defined by requiring $-0.2<\cos \theta_{l}^{*}<1$. In section 8 , this sample is used to fit the branching ratio $\mathcal{B}\left(t \rightarrow b H^{+}\right)$and the product of the cross section $\sigma_{b b W W}$, the luminosity, the selection efficiency and acceptance for $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$, simultaneously with the likelihood for the signal estimation. In turn, this ensures that the final results, and in particular the upper limit on $\mathcal{B}\left(t \rightarrow b H^{+}\right)$, are independent of the assumed theoretical production cross section for $t \bar{t}$. With a branching fraction $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$, the signal contamination in the control region would range from $1.3 \%$ for $m_{H^{+}}=90 \mathrm{GeV}$ to $0.4 \%$ for $m_{H^{+}}=160 \mathrm{GeV}$. The signal region is defined by requiring $\cos \theta_{l}^{*}<-0.6$ and $m_{\mathrm{T}}^{W}<60 \mathrm{GeV}$, where:

$$
\begin{equation*}
m_{\mathrm{T}}^{W}=\sqrt{2 p_{\mathrm{T}}^{l} E_{\mathrm{T}}^{\mathrm{miss}}\left(1-\cos \Delta \phi_{l, \mathrm{miss}}\right)} . \tag{4.8}
\end{equation*}
$$

This is done in order to suppress the background from events with a $W$ boson decaying directly into electrons or muons. For events in the signal region, $m_{\mathrm{T}}^{H}$, shown in figure 2 b , is used as a discriminating variable to search for charged Higgs bosons. Table 2 lists the contributions to the signal region of the SM processes and of $t \bar{t}$ events with at least one decay $t \rightarrow b H^{+}$, assuming $m_{H^{+}}=130 \mathrm{GeV}$ and $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$. When including signal in the prediction, the simulated SM $t \bar{t}$ contribution is scaled according to this branching ratio. The data are consistent with the predicted SM background and no significant deformation of the $m_{\mathrm{T}}^{H}$ distribution is observed.

| Sample | Event yield (lepton+jets) |  |  |
| :--- | :---: | :--- | :--- |
| $t \bar{t}$ | 840 | $\pm 20$ | $\pm 150$ |
| Single top quark | 28 | $\pm 2$ | ${ }_{-6}^{+8}$ |
| $W+$ jets | 14 | $\pm 3$ | ${ }_{-3}^{+6}$ |
| $Z+$ jets | 2.1 | $\pm 0.7$ | ${ }_{-0.4}^{+1.2}$ |
| Diboson | 0.5 | $\pm 0.1$ | $\pm 0.2$ |
| Misidentified leptons | 55 | $\pm 10$ | $\pm 20$ |
| All SM backgrounds | 940 | $\pm 22$ | $\pm 150$ |
| Data | 933 |  |  |
| $t \rightarrow b H^{+}(130 ~ G e V)$ | 120 | $\pm 4$ | $\pm 25$ |
| Signal+background | 990 | $\pm 21 \pm 140$ |  |

Table 2. Expected event yields in the signal region of the lepton+jets final state, and comparison with $4.6 \mathrm{fb}^{-1}$ of data. A cross section of 167 pb is assumed for the $\mathrm{SM} t \bar{t}$ background. The numbers shown in the last two rows, for a hypothetical $H^{+}$signal with $m_{H^{+}}=130 \mathrm{GeV}$, are obtained with $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$. Both statistical and systematic uncertainties are shown, in this order.

(a)

(b)

Figure 2. Distribution of (a) $\cos \theta_{l}^{*}$ and (b) $m_{\mathrm{T}}^{H}$, in the signal region ( $\cos \theta_{l}^{*}<-0.6, m_{\mathrm{T}}^{W}<60 \mathrm{GeV}$ ) for the latter. The dashed line corresponds to the SM-only hypothesis and the hatched area around it shows the total uncertainty for the SM backgrounds, where "Others" refers to the contribution of all SM processes except $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$. The solid line shows the predicted contribution of signal+background in the presence of a 130 GeV charged Higgs boson, assuming $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$ and $\mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)=100 \%$. The light area below the solid line corresponds to the contribution of the $H^{+}$signal, stacked on top of the scaled $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$background and other SM processes.

## 5 Analysis of the $\tau+$ lepton channel

This analysis relies on the detection of $\tau+$ lepton decays of $t \bar{t}$ events, where the hadronically decaying $\tau$ lepton arises from $H^{+} \rightarrow \tau_{\text {had }} \nu$, while an electron or muon comes from the decay of the $W$ boson, i.e. $t \bar{t} \rightarrow b \bar{b} W H^{+} \rightarrow b \bar{b}(l \nu)\left(\tau_{\text {had }} \nu\right)$.

### 5.1 Event selection

The $\tau+$ lepton analysis relies on the same single-lepton trigger signatures as the lepton+jets analysis presented in section 4. In order to select $\tau+$ lepton events, the following requirements are made:

- exactly one lepton, having $E_{\mathrm{T}}>25 \mathrm{GeV}$ (electron) or $p_{\mathrm{T}}>20 \mathrm{GeV}$ (muon) and matched to the corresponding trigger object, and no other electron or muon;
- exactly one $\tau$ jet having $p_{\mathrm{T}}>20 \mathrm{GeV}$ and an electric charge opposite to that of the lepton;
- at least two jets having $p_{\mathrm{T}}>20 \mathrm{GeV}$, including at least one $b$-tagged jet;
- $\sum p_{\mathrm{T}}>100 \mathrm{GeV}$ in order to suppress multi-jet events, where $\sum p_{\mathrm{T}}$ is the sum of the transverse momenta of all tracks associated with the primary vertex. Tracks entering the sum must pass quality cuts on the number of hits and have $p_{\mathrm{T}}>1 \mathrm{GeV}$. As this variable is based on tracks from the primary vertex (as opposed to energy deposits in the calorimeter), it is robust against pile-up.
$E_{\mathrm{T}}^{\text {miss }}$ is used as the discriminating variable to distinguish between SM $t \bar{t}$ events and those where top quark decays are mediated by a charged Higgs boson, in which case the neutrinos are likely to carry away more energy.


### 5.2 Data-driven estimation of backgrounds with misidentified leptons

The estimation of the backgrounds with misidentified leptons uses the data-driven method described in section 4.2. When implementing the method, the dependence of real and misidentification rates on the $b$-tagged jet multiplicity are taken into account, as well as the requirement for one $\tau$ jet (instead of a $\tau$ jet veto).

### 5.3 Backgrounds with electrons and jets misidentified as $\tau$ jets

The background with electrons misidentified as $\tau$ jets is estimated using a $Z \rightarrow e e$ control region in the data [51], where one electron is reconstructed as a $\tau$ jet. The measured misidentification probabilities, which have an average value of $0.2 \%$, are then applied to all simulated events in the $\tau+$ lepton analysis. Simulation studies show that this application is valid, as the misidentification probabilities for $Z \rightarrow e e$ and $t \bar{t}$ events are similar.

A data-driven method applied to a control sample enriched in $W+$ jets events is used to measure the probability for a jet to be misidentified as a hadronically decaying $\tau$ lepton. This measured probability is used to predict the yield of background events due to jet $\rightarrow \tau$ misidentification. Like jets from the hard process in the dominant $t \bar{t}$ background, jets in the
control sample originate predominantly from quarks instead of gluons. The main difference between $t \bar{t}$ and $W+$ jets events is the different fraction of $b$ jets, which is smaller in $W+$ jets events. However, the probability for a $b$ jet to be misidentified as a $\tau$ jet is smaller than the corresponding probability for a light-quark jet, because the average track multiplicity is higher for $b$ jets. Moreover, the visible mass measurement used in the $\tau$ identification provides further discrimination between $b$ jets and $\tau$ jets. Differences in jet composition (e.g. the ratio of gluons to quarks) between $t \bar{t}$ and $W+$ jets, assessed using simulation, are taken into account as systematic uncertainties. These also cover the dependence of the probability on whether a $b$ jet or a light-quark jet is misidentified as a $\tau$ jet. Events in the control region are required to pass the same single-lepton trigger, data quality and lepton requirements as in the $\tau+$ lepton event selection. Additionally, a $\tau$ candidate and $E_{\mathrm{T}}^{\mathrm{miss}}>40 \mathrm{GeV}$ are required, and events with $b$-tagged jets are vetoed. Simulated events with a true $\tau$ contribute at a level below $0.5 \%$ and are subtracted. The $\tau$ candidates are required to have $p_{\mathrm{T}}>20 \mathrm{GeV},|\eta|<2.3$, and cannot be within $\Delta R=0.2$ of any electron or muon. They are also not required to pass $\tau$ identification. The jet $\rightarrow \tau$ misidentification probability is defined as the number of objects passing the full $\tau$ identification divided by the number prior to requiring identification. This misidentification probability is evaluated separately for $\tau$ candidates with one or three associated tracks (the corresponding average values are about $7 \%$ and $2 \%$, respectively) and, in addition, it is measured as a function of both $p_{\mathrm{T}}$ and $\eta$.

In order to predict the background for the charged Higgs boson search, the measured jet $\rightarrow \tau$ misidentification probability is applied to simulated $t \bar{t}$, single top quark, $W+$ jets, $Z / \gamma^{*}+$ jets and diboson events, all of which are required to pass the full event selection except for the $\tau$ identification. For these events, $\tau$ candidates not overlapping with a true $\tau$ lepton or a true electron, but otherwise fulfilling the same requirements as in the denominator of the misidentification probability, are identified. Each of them is considered separately to be potentially misidentified as a $\tau$ jet. In order to avoid counting the same object twice, each jet that corresponds to a $\tau$ candidate is removed from the event. The number of reconstructed jets and the number of $b$-tagged jets are adjusted accordingly. If, after taking this into consideration, the event passes the $\tau+$ lepton selection, it is counted as a background event with a weight given by the misidentification probability corresponding to the $p_{\mathrm{T}}$ and $\eta$ of the $\tau$ candidate. The predicted numbers of events from this datadriven method and from simulation are shown in table 3. The backgrounds arising from the jet $\rightarrow \tau$ misidentification are not well modelled in simulation, which is why they are estimated using data-driven methods.

### 5.4 Event yields and $E_{\mathrm{T}}^{\text {miss }}$ distribution after the selection cuts

Table 4 shows the expected number of background events for the SM-only hypothesis and the observation in the data. The total number of predicted events (signal+background) in the presence of a 130 GeV charged Higgs boson with $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$ is also shown. The $\tau+$ lepton analysis relies on the theoretical $t \bar{t}$ production cross section $\sigma_{t \bar{t}}=167_{-18}^{+17} \mathrm{pb}[26]$ for the background estimation. In the presence of a charged Higgs boson in the top quark decays, with a branching ratio $\mathcal{B}\left(t \rightarrow b H^{+}\right)$, the contributions of $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$events in the backgrounds with true or misidentified $\tau$ jets are scaled according to this branching

| Sample | Data-driven method [events] | Simulation [events] |
| :--- | :---: | :---: |
| $t \bar{t}$ | $900 \pm 15$ | $877 \pm 6$ |
| $W+$ jets | $150 \pm 3$ | $145 \pm 9$ |
| Single top quark | $81 \pm 1$ | $61 \pm 2$ |
| $Z / \gamma^{*}+$ jets | $44 \pm 1$ | $69 \pm 4$ |
| Diboson | $6 \pm 1$ | $8 \pm 1$ |

Table 3. Application of the misidentification probability obtained from $W+$ jets events in the data, for the $\tau+$ lepton channel. The predictions of the background contributions based on data-driven misidentification probabilities and on simulation are given, with statistical uncertainties only. In both cases, all top quarks are assumed to decay via $t \rightarrow b W$.

| Sample | Event yield ( $\tau+$ lepton) |  |
| :--- | ---: | ---: |
|  | $\tau+e$ | $\tau+\mu$ |
| True $\tau+$ lepton | $430 \pm 14 \pm 59$ | $570 \pm 15 \pm 75$ |
| Misidentified jet $\rightarrow \tau$ | $510 \pm 23 \pm 86$ | $660 \pm 26 \pm 110$ |
| Misidentified $e \rightarrow \tau$ | $33 \pm 4 \pm$ | 5 |
| Misidentified leptons | $39 \pm 4 \pm \pm$ | 6420 |
| All SM backgrounds | $1010 \pm 30 \pm 110$ | $1360 \pm 30 \pm 140$ |
| Data | 880 | 1219 |
| $t \rightarrow b H^{+}(130 \mathrm{GeV})$ | $220 \pm 6 \pm 29$ | $310 \pm 7 \pm 39$ |
| Signal+background | $1160 \pm 30 \pm 100$ | $1570 \pm 30 \pm 130$ |

Table 4. Expected event yields after all selection cuts in the $\tau+l$ lepton channel and comparison with $4.6 \mathrm{fb}^{-1}$ of data. The numbers in the last two rows, obtained for a hypothetical $H^{+}$signal with $m_{H^{+}}=130 \mathrm{GeV}$, are obtained with $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$. All other rows assume $\mathcal{B}(t \rightarrow b W)=100 \%$. Both statistical and systematic uncertainties are shown, in this order.
ratio. The background with correctly reconstructed $\tau$ jets is obtained with simulation. The data are found to be consistent with the expectation for the background-only hypothesis. The $E_{\mathrm{T}}^{\text {miss }}$ distributions for the $\tau+e$ and $\tau+\mu$ channels, after all selection cuts are applied, are shown in figure 3 .

## 6 Analysis of the $\tau+$ jets channel

The analysis presented here relies on the detection of $\tau+$ jets decays of $t \bar{t}$ events, where the hadronically decaying $\tau$ lepton arises from $H^{+} \rightarrow \tau_{\text {had }} \nu$, while the jets come from a hadronically decaying $W$ boson, i.e. $t \bar{t} \rightarrow b \bar{b} W H^{+} \rightarrow b \bar{b}\left(q \bar{q}^{\prime}\right)\left(\tau_{\text {had }} \nu\right)$.


Figure 3. $E_{\mathrm{T}}^{\text {miss }}$ distribution after all selection cuts in the $\tau+$ lepton channel, for (a) $\tau+$ electron and (b) $\tau+$ muon final states. The dashed line corresponds to the SM-only hypothesis and the hatched area around it shows the total uncertainty for the SM backgrounds. The solid line shows the predicted contribution of signal+background in the presence of a 130 GeV charged Higgs boson with $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$ and $\mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)=100 \%$. The contributions of $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$events in the backgrounds with true or misidentified $\tau$ jets are scaled down accordingly.

### 6.1 Event selection

The $\tau+$ jets analysis uses events passing a $\tau+E_{\mathrm{T}}^{\mathrm{miss}}$ trigger with a threshold of 29 GeV on the $\tau$ object and 35 GeV on calorimeter-based $E_{\mathrm{T}}^{\mathrm{miss}}$. The following requirements are applied, in this order:

- at least four jets (excluding $\tau$ jets) having $p_{\mathrm{T}}>20 \mathrm{GeV}$, of which at least one is b-tagged;
- exactly one $\tau$ jet with $p_{\mathrm{T}}^{\tau}>40 \mathrm{GeV}$, found within $|\eta|<2.3$ and matched to a $\tau$ trigger object;
- neither a second $\tau$ jet with $p_{\mathrm{T}}^{\tau}>20 \mathrm{GeV}$, nor any electrons with $E_{\mathrm{T}}>20 \mathrm{GeV}$, nor any muons with $p_{\mathrm{T}}>15 \mathrm{GeV}$;
- $E_{\mathrm{T}}^{\mathrm{miss}}>65 \mathrm{GeV}$;
- to reject events in which a large reconstructed $E_{\mathrm{T}}^{\mathrm{miss}}$ is due to the limited resolution of the energy measurement, the following ratio based on the $\sum p_{\mathrm{T}}$ definition of section 5 must satisfy:

$$
\frac{E_{\mathrm{T}}^{\mathrm{miss}}}{0.5 \mathrm{GeV}^{1 / 2} \cdot \sqrt{\sum p_{\mathrm{T}}}}>13
$$

- a topology consistent with a top quark decay: the combination of one $b$-tagged jet ( $b$ ) and two untagged jets $(j)$ with the highest $p_{\mathrm{T}}^{j j b}$ must satisfy $m_{j j b} \in[120,240] \mathrm{GeV}$.

For the selected events, the transverse mass $m_{\mathrm{T}}$ is defined as:

$$
\begin{equation*}
m_{\mathrm{T}}=\sqrt{2 p_{\mathrm{T}}^{\tau} E_{\mathrm{T}}^{\mathrm{miss}}\left(1-\cos \Delta \phi_{\tau, \mathrm{miss}}\right)} \tag{6.1}
\end{equation*}
$$

where $\Delta \phi_{\tau, \text { miss }}$ is the azimuthal angle between the $\tau$ jet and the direction of the missing momentum. This discriminating variable is related to the $W$ boson mass in the $W \rightarrow \tau \nu$ background case and to the $H^{+}$mass for the signal hypothesis.

### 6.2 Data-driven estimation of the multi-jet background

The multi-jet background is estimated by fitting its $E_{\mathrm{T}}^{\mathrm{miss}}$ shape (and the $E_{\mathrm{T}}^{\mathrm{miss}}$ shape of other backgrounds) to data. In order to study this shape in a data-driven way, a control region is defined where the $\tau$ identification and $b$-tagging requirements are modified, i.e. $\tau$ candidates must pass a loose $\tau$ identification but fail the tight $\tau$ identification used in the signal selection, and the event is required not to contain any $b$-tagged jet. Hence, the requirement on $m_{j j b}$ is also removed. Assuming that the shapes of the $E_{\mathrm{T}}^{\text {miss }}$ and $m_{\mathrm{T}}$ distributions are the same in the control and signal regions, the $E_{\mathrm{T}}^{\mathrm{miss}}$ shape for the multi-jet background is measured in the control region, after subtracting the simulated background contributions from other processes. These other processes amount to less than $1 \%$ of the observed events in the control region. The $E_{\mathrm{T}}^{\mathrm{miss}}$ shapes obtained with the $\tau+$ jets selection of section 6.1 or in the control region are compared just before the $E_{\mathrm{T}}^{\mathrm{miss}}$ requirement in the baseline selection in figure 4a. The differences between the two distributions are accounted for as systematic uncertainties. For the baseline selection, the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution measured in the data is then fit using two shapes: the multi-jet model and the sum of other processes (dominated by $t \bar{t}$ and $W+$ jets), for which the shape and the relative normalisation are taken from simulation, as shown in figure 4 b . The ratio between the numbers of multi-jet background events in the control and signal regions enters the likelihood function for the signal estimation (see section 8) as a nuisance parameter while the shape of the multi-jet background is measured in the same region after additionally requiring $E_{\mathrm{T}}^{\mathrm{miss}}>65 \mathrm{GeV}$.

### 6.3 Backgrounds with electrons and jets misidentified as $\tau$ jets

The methods described in section 5.3 are used to estimate the probability for electrons or jets to be misidentified as $\tau$ jets. The estimated contribution to the background from the jet $\rightarrow \tau$ misidentification after the $\tau+$ jets selection is given in table 5 . The backgrounds arising from the jet $\rightarrow \tau$ misidentification are not expected to be well modelled in simulation, which is why they are estimated using data-driven methods.

### 6.4 Data-driven estimation of backgrounds with correctly reconstructed $\tau$ jets

An embedding method [54] is used to estimate the backgrounds that contain correctly reconstructed $\tau$ jets. The method consists of selecting a control sample of $t \bar{t}$-like $\mu+$ jets events and replacing the detector signature of the muon by a simulated hadronic $\tau$ decay. These new hybrid events are then used for the background prediction. In order to select this control sample from the data, the following event selection is applied:

- event triggered by a single-muon trigger with a $p_{\mathrm{T}}$ threshold of 18 GeV ;


Figure 4. (a) Shape of $E_{\mathrm{T}}^{\mathrm{miss}}$ in a control region of the data or using the baseline selection, after subtracting the expectation from $t \bar{t}, W+$ jets, and single top quark processes estimated from simulation. The distributions are compared just before the $E_{\mathrm{T}}^{\text {miss }}$ requirement in the baseline selection of section 6.1, with the exception that, in the control region, the $\tau$ selection and the $b$-tagging requirements are modified, see text. (b) Fit of the $E_{\mathrm{T}}^{\text {miss }}$ template to data, in the signal region. Only statistical uncertainties are shown.

| Sample | Data-driven method [events] | Simulation [events] |
| :--- | :---: | :---: |
| $t \bar{t}$ | $33 \pm 1$ | $37 \pm 1$ |
| $W+$ jets | $2.5 \pm 0.1$ | $3.9 \pm 1.5$ |
| Single top quark | $1.3 \pm 0.1$ | $2.0 \pm 0.3$ |

Table 5. Application of the misidentification probability obtained from a control region in the data enriched in $W+$ jets events, for the $\tau+$ jets channel. The predictions of the background contributions based on data-driven misidentification probabilities and on simulation are given, with statistical uncertainties only. In both cases, all top quarks decay via $t \rightarrow b W$.

- exactly one isolated muon with $p_{\mathrm{T}}>25 \mathrm{GeV}$, no isolated electron with $E_{\mathrm{T}}>20 \mathrm{GeV}$;
- at least four jets with $p_{\mathrm{T}}>20 \mathrm{GeV}$, at least one of which is $b$-tagged;
- $E_{\mathrm{T}}^{\mathrm{miss}}>35 \mathrm{GeV}$.

This selection is looser than the selection defined in section 6.1 in order not to bias the control sample. The impurity from the background with muons produced in $\tau$ decays and non-isolated muons (dominantly $b \bar{b}$ and $c \bar{c}$ events) is about $10 \%$. However, this contribution is greatly reduced as these events are much less likely to pass the $\tau+$ jets selection, in particular the $p_{\mathrm{T}}^{\tau}$ requirement.

The shape of the $m_{\mathrm{T}}$ distribution for the backgrounds with true $\tau$ jets is taken from the distribution obtained with the embedded events, after having applied the $\tau+$ jets event selection. The normalisation is then derived from the number of embedded events:

$$
\begin{equation*}
N_{\tau}=N_{\text {embedded }} \cdot\left(1-c_{\tau \rightarrow \mu}\right) \frac{\epsilon^{\tau+E_{\mathrm{T}}^{\text {miss }}-\text { trigger }}}{\epsilon^{\mu-\mathrm{ID}, \text { trigger }}} \cdot \mathcal{B}(\tau \rightarrow \text { hadrons }+\nu), \tag{6.2}
\end{equation*}
$$



Figure 5. Comparison of the $m_{\mathrm{T}}$ distribution for correctly reconstructed $\tau$ jets, predicted by the embedding method and simulation. Combined statistical and systematic uncertainties (as described in section 7) are shown.
where $N_{\tau}$ is the estimated number of events with correctly reconstructed $\tau$ jets, $N_{\text {embedded }}$ is the number of embedded events in the signal region, $c_{\tau \rightarrow \mu}$ is the fraction of events in which the selected muon is a decay product of a $\tau$ lepton (taken from simulation), $\epsilon^{\tau+E_{\mathrm{T}}^{\text {miss }} \text {-trigger }}$ is the $\tau+E_{\mathrm{T}}^{\mathrm{miss}}$ trigger efficiency (as a function of $p_{T}^{\tau}$ and $E_{\mathrm{T}}^{\text {miss }}$, derived from data), $\epsilon^{\mu-\mathrm{ID}, \text { trigger }}$ is the muon trigger and identification efficiency (as a function of $p_{T}$ and $\eta$, derived from data) and $\mathcal{B}(\tau \rightarrow$ hadrons $+\nu)$ is the branching ratio of the $\tau$ lepton decays involving hadrons. The $m_{\mathrm{T}}$ distribution for correctly reconstructed $\tau$ jets, as predicted by the embedding method, is shown in figure 5 and compared to simulation.

### 6.5 Event yields and $m_{\mathrm{T}}$ distribution after the selection cuts

Table 6 shows the expected number of background events for the SM-only hypothesis and the observation in the data. The total number of predicted events (signal+background) in the presence of a 130 GeV charged Higgs boson with $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$ is also shown. The number of events with a correctly reconstructed $\tau$ jet is derived from the number of embedded events and does not depend on the cross section of the $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$process. On the other hand, the $\tau+$ jets analysis relies on the theoretical inclusive $t \bar{t}$ production cross section $\sigma_{t \bar{t}}=167_{-18}^{+17} \mathrm{pb}[26]$ for the estimation of the background with electrons or jets misidentified as $\tau$ jets. In the presence of a charged Higgs boson in the top quark decays, with a branching ratio $\mathcal{B}\left(t \rightarrow b H^{+}\right)$, the contributions of $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$events in these backgrounds are scaled according to this branching ratio. The data are found to be consistent with the estimation of the SM background. The $m_{\mathrm{T}}$ distribution for the $\tau+$ jets channel, after all selection cuts are applied, is shown in figure 6.

| Sample | Event yield $(\tau+$ jets $)$ |
| :--- | :---: |
| True $\tau$ (embedding method) | $210 \pm 10 \pm 44$ |
| Misidentified jet $\rightarrow \tau$ | $36 \pm 6 \pm 10$ |
| Misidentified $e \rightarrow \tau$ | $3 \pm 1 \pm 1$ |
| Multi-jet processes | $74 \pm 3 \pm 47$ |
| All SM backgrounds | $330 \pm 12 \pm 65$ |
| Data | 355 |
| $t \rightarrow b H^{+}(130 \mathrm{GeV})$ | $220 \pm 6 \pm 56$ |
| Signal + background | $540 \pm 13 \pm 85$ |

Table 6. Expected event yields after all selection cuts in the $\tau+$ jets channel and comparison with $4.6 \mathrm{fb}^{-1}$ of data. The numbers in the last two rows, obtained for a hypothetical $H^{+}$signal with $m_{H^{+}}=130 \mathrm{GeV}$, are obtained with $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$. The rows for the backgrounds with misidentified objects assume $\mathcal{B}(t \rightarrow b W)=100 \%$. Both statistical and systematic uncertainties are shown, in this order.


Figure 6. Distribution of $m_{\mathrm{T}}$ after all selection cuts in the $\tau+$ jets channel. The dashed line corresponds to the SM-only hypothesis and the hatched area around it shows the total uncertainty for the SM backgrounds. The solid line shows the predicted contribution of signal + background in the presence of a charged Higgs boson with $m_{H^{+}}=130 \mathrm{GeV}$, assuming $\mathcal{B}\left(t \rightarrow b H^{+}\right)=5 \%$ and $\mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)=100 \%$. The contributions of $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$events in the backgrounds with misidentified objects are scaled down accordingly.

## $7 \quad$ Systematic uncertainties

### 7.1 Systematic uncertainties arising from the detector simulation

Systematic uncertainties arising from the simulation of pile-up and object reconstruction are considered. The latter arise from the simulation of the trigger, from the reconstruction and identification efficiencies, as well as from the energy/momentum scale and resolution for the objects described in section 3. To assess the impact of most sources of systematic uncertainty, the selection cuts for each analysis are re-applied after shifting a particular parameter by its $\pm 1$ standard deviation uncertainty. The systematic uncertainties related to the electrons and muons are discussed in, respectively, ref. [42] and refs. [43, 55]. For the jets, see ref. [48] and, in particular, ref. [50] for the b-tagging calibration. The systematic uncertainties related to $\tau$ jets are discussed in ref. [51]. Finally, for the reconstruction of $E_{\mathrm{T}}^{\mathrm{miss}}$, see ref. [52]. All studies of systematic uncertainties have been updated with the full dataset collected in 2011. The dominant instrumental systematic uncertainties arise from the jet energy resolution ( $10-30 \%$, depending on $p_{\mathrm{T}}$ and $\eta$ ), the jet energy scale (up to $14 \%$, depending on $p_{\mathrm{T}}$ and $\eta$, to which a pile-up term of $2-7 \%$ and a $b$ jet term of $2.5 \%$ are added in quadrature), as well as the $b$-tagging efficiency ( $5-17 \%$, depending on $p_{\mathrm{T}}$ and $\eta$ ) and misidentification probability ( $12-21 \%$, depending on $p_{\mathrm{T}}$ and $\eta$ ). In comparison, the systematic uncertainties arising from the reconstruction and identification of electrons and muons are small. All instrumental systematic uncertainties are also propagated to the reconstructed $E_{\mathrm{T}}^{\mathrm{miss}}$.

### 7.2 Systematic uncertainties arising from the generation of $t \bar{t}$ events

In order to estimate the systematic uncertainties arising from the $t \bar{t}$ generation and the parton shower model, the acceptance is computed for $t \bar{t}$ events produced with MC@NLO interfaced to HERWIG/JIMMY and POWHEG [56] interfaced to PYTHIA. For the signal samples, which are generated with PYTHIA (i.e. without higher-order corrections), no alternative generator is available. Instead, the systematic uncertainty for the signal samples is set to the relative difference in acceptance between $t \bar{t}$ events generated with MC@NLO interfaced to HERWIG/JIMMY and with AcerMC, which is also a leading-order generator, interfaced to PYTHIA. The systematic uncertainties arising from initial and final state radiation are computed using $t \bar{t}$ samples generated with AcerMC interfaced to PYTHIA, where initial and final state radiation parameters are set to a range of values not excluded by the experimental data [57]. The largest relative differences with respect to the reference sample after full event selections are used as systematic uncertainties. The systematic uncertainties arising from the modelling of the $t \bar{t}$ event generation and the parton shower, as well as initial and final state radiation, are summarised in table 7 for each analysis.

### 7.3 Systematic uncertainties arising from data-driven background estimates

The systematic uncertainties arising from the data-driven methods used to estimate the various backgrounds are summarised in table 8 , for each of the three channels considered in the analysis.

| Source of uncertainty | Normalisation uncertainty |
| :--- | ---: |
| lepton+jets: |  |
| Generator and parton shower $\left(b \bar{b} W H^{+}\right.$, signal region) | $10 \%$ |
| Generator and parton shower $\left(b \bar{b} W^{+} W^{-}\right.$, signal region) | $8 \%$ |
| Generator and parton shower $\left(b \bar{b} W H^{+}\right.$, control region) | $7 \%$ |
| Generator and parton shower $\left(b \bar{b} W^{+} W^{-}\right.$, control region) | $6 \%$ |
| Initial and final state radiation (signal region) | $8 \%$ |
| Initial and final state radiation (control region) | $13 \%$ |
| $\tau+$ lepton: |  |
| Generator and parton shower $\left(b \bar{b} W H^{+}\right)$ | $2 \%$ |
| Generator and parton shower $\left(b \bar{b} W^{+} W^{-}\right)$ | $5 \%$ |
| Initial and final state radiation | $13 \%$ |
| $\tau+$ jets: |  |
| Generator and parton shower $\left(b \bar{b} W H^{+}\right)$ | $5 \%$ |
| Generator and parton shower $\left(b \bar{b} W W^{+} W^{-}\right)$ | $5 \%$ |
| Initial and final state radiation | $19 \%$ |

Table 7. Systematic uncertainties arising from the modelling of $t \bar{t} \rightarrow b \bar{b} W^{+} W^{-}$and $t \bar{t} \rightarrow b \bar{b} W H^{+}$ events and the parton shower, as well as from initial and final state radiation.

For backgrounds with misidentified leptons, discussed in sections 4.2 and 5.2 , the main systematic uncertainties arise from the simulated samples used for subtracting true leptons in the determination of the misidentification probabilities. These are sensitive to the instrumental systematic uncertainties and to the sample dependence (misidentification probabilities are calculated in a control region dominated by gluon-initiated events, but later used in a data sample with a higher fraction of quark-initiated events).

The dominant systematic uncertainties in the estimation of the multi-jet background in the $\tau+$ jets channel, described in section 6.2, are the statistical uncertainty of the fit due to the limited size of the data control sample and uncertainties due to potential differences of the $E_{\mathrm{T}}^{\text {miss }}$ shape in the signal and control regions. The dominant systematic uncertainties in estimating the contribution of events with electrons misidentified as $\tau$ jets in sections 5.3 and 6.3 arise from the subtraction of the multi-jet and electroweak backgrounds in the control region enriched with $Z \rightarrow e e$ events and from potential correlations in the selections of the tag and probe electrons. For the estimation of backgrounds with jets misidentified as hadronically decaying $\tau$ leptons, also discussed in sections 5.3 and 6.3 , the dominant systematic uncertainties on the misidentification probability are the statistical uncertainty due to the limited control sample size and uncertainties due to the difference of the jet composition (gluon- or quark-initiated) in the control and signal regions, which is estimated

| Source of uncertainty | Normalisation uncertainty | Shape uncertainty |
| :---: | :---: | :---: |
| lepton+jets: lepton misidentification |  |  |
| Choice of control region | 6\% | - |
| $Z$ mass window | $4 \%$ | - |
| Jet energy scale | 16\% | - |
| Jet energy resolution | 7\% | - |
| Sample composition | $31 \%$ | - |
| $\tau+$ lepton: jet $\rightarrow \tau$ misidentification |  |  |
| Statistics in control region | 2\% | - |
| Jet composition | 11\% | - |
| Object-related systematics | 23\% | $3 \%$ |
| $\tau+$ lepton: $e \rightarrow \tau$ misidentification |  |  |
| Misidentification probability | 20\% | - |
| $\tau+$ lepton: lepton misidentification |  |  |
| Choice of control region | $4 \%$ | - |
| $Z$ mass window | 5\% | - |
| Jet energy scale | $14 \%$ | - |
| Jet energy resolution | 4\% | - |
| Sample composition | 39\% | - |
| $\tau+$ jets: true $\tau$ |  |  |
| Embedding parameters | 6\% | 3\% |
| Muon isolation | 7\% | $2 \%$ |
| Parameters in normalisation | 16\% | - |
| $\tau$ identification | 5\% | - |
| $\tau$ energy scale | 6\% | 1\% |
| $\tau+$ jets: jet $\rightarrow \tau$ misidentification |  |  |
| Statistics in control region | 2\% | - |
| Jet composition | 12\% | - |
| Purity in control region | 6\% | 1\% |
| Object-related systematics | 21\% | $2 \%$ |
| $\tau+$ jets: $e \rightarrow \tau$ misidentification |  |  |
| Misidentification probability | 22\% | - |
| $\tau+$ jets: multi-jet estimate |  |  |
| Fit-related uncertainties | $32 \%$ | - |
| $E_{\mathrm{T}}^{\text {miss }}$-shape in control region | 16\% | - |

Table 8. Dominant systematic uncertainties on the data-driven estimates. The shape uncertainty given is the relative shift of the mean value of the final discriminant distribution. A "-" in the second column indicates negligible shape uncertainties.
using simulation. Other uncertainties come from the impurities arising from multi-jet background events and from true hadronic $\tau$ decays in the control sample. The systematic uncertainties affecting the estimation of the background from correctly reconstructed $\tau$ jets in the $\tau+$ jets channel, discussed in section 6.4 , consist of the potential bias introduced by the embedding method itself, uncertainties from the trigger efficiency measurement, uncertainties associated to simulated $\tau$ jets ( $\tau$ energy scale and identification efficiency) and uncertainties on the normalisation, which are dominated by the statistical uncertainty of the selected control sample and the $\tau+E_{\mathrm{T}}^{\text {miss }}$ trigger efficiency uncertainties.

## 8 Results

In order to test the compatibility of the data with background-only and signal+background hypotheses, a profile likelihood ratio [58] is used with $m_{\mathrm{T}}^{H}$ (lepton+jets), $E_{\mathrm{T}}^{\text {miss }}$ ( $\tau+$ lepton) and $m_{\mathrm{T}}(\tau+$ jets $)$ as the discriminating variables. The statistical analysis is based on a binned likelihood function for these distributions. The systematic uncertainties in shape and normalisation are incorporated via nuisance parameters, and the one-sided profile likelihood ratio, $\tilde{q}_{\mu}$, is used as a test statistic. No significant deviation from the SM prediction is observed in any of the investigated final states in $4.6 \mathrm{fb}^{-1}$ of data. Exclusion limits are set on the branching fraction $\mathcal{B}\left(t \rightarrow b H^{+}\right)$and, in the context of the $m_{h}^{\max }$ scenario of the MSSM, on $\tan \beta$, by rejecting the signal hypothesis at the $95 \%$ confidence level (CL) using the $\mathrm{CL}_{s}$ procedure [59]. These limits are based on the asymptotic distribution of the test statistic [58]. The combined limit is derived from the product of the individual likelihoods, and systematic uncertainties are treated as correlated where appropriate. The exclusion limits for the individual channels, as well as the combined limit, are shown in figure 7 in terms of $\mathcal{B}\left(t \rightarrow b H^{+}\right)$with the assumption $\mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)=100 \%$. In figure 8 , the combined limit on $\mathcal{B}\left(t \rightarrow b H^{+}\right) \times \mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)$ is interpreted in the context of the $m_{h}^{\max }$ scenario of the MSSM. The following relative theoretical uncertainties on $\mathcal{B}\left(t \rightarrow b H^{+}\right)$are considered [60, 61]:5\% for one-loop electroweak corrections missing from the calculations, $2 \%$ for missing two-loop QCD corrections, and about $1 \%$ (depending on $\tan \beta$ ) for $\Delta_{b}$-induced uncertainties, where $\Delta_{b}$ is a correction factor to the running $b$ quark mass [62]. These uncertainties are added linearly, as recommended by the LHC Higgs cross section working group [61].

## 9 Conclusions

Charged Higgs bosons have been searched for in $t \bar{t}$ events, in the decay mode $t \rightarrow b H^{+}$followed by $H^{+} \rightarrow \tau \nu$. For this purpose, a total of $4.6 \mathrm{fb}^{-1}$ of $p p$ collision data at $\sqrt{s}=7 \mathrm{TeV}$, recorded in 2011 with the ATLAS experiment, is used. Three final states are considered, which are characterised by the presence of a leptonic or hadronic $\tau$ decay, $E_{\mathrm{T}}^{\mathrm{miss}}, b$ jets, and a leptonically or hadronically decaying $W$ boson. Data-driven methods and simulation are employed to estimate the number of background events. The observed data are found to be in agreement with the SM predictions. Assuming $\mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)=100 \%$, upper limits at the $95 \%$ confidence level have been set on the branching ratio $\mathcal{B}\left(t \rightarrow b H^{+}\right)$between $5 \%\left(m_{H^{+}}=90 \mathrm{GeV}\right)$ and $1 \%\left(m_{H^{+}}=160 \mathrm{GeV}\right)$. This result constitutes a significant


Figure 7. Expected and observed $95 \%$ CL exclusion limits on $\mathcal{B}\left(t \rightarrow b H^{+}\right)$for charged Higgs boson production from top quark decays as a function of $m_{H^{+}}$, assuming $\mathcal{B}\left(H^{+} \rightarrow \tau \nu\right)=100 \%$. Shown are the results for: (a) lepton+jets channel; (b) $\tau+$ lepton channel; (c) $\tau+$ jets channel; (d) combination.
improvement compared to existing limits provided by the Tevatron experiments [14, 15] over the whole investigated mass range, but in particular for $m_{H^{+}}$close to the top quark mass. Interpreted in the context of the $m_{h}^{\max }$ scenario of the MSSM, $\tan \beta$ above 12-26, as well as between 1 and 2-6, can be excluded in the mass range $90 \mathrm{GeV}<m_{H^{+}}<150 \mathrm{GeV}$.

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Figure 8．Combined $95 \%$ CL exclusion limits on $\tan \beta$ as a function of $m_{H^{+}}$．Results are shown in the context of the MSSM scenario $m_{h}^{\max }$ for the region $1<\tan \beta<60$ in which reliable theoretical predictions exist．The theoretical uncertainties described in the text are shown as well．

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Link model simulation and power penalty specification of the versatile link systems

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# Link model simulation and power penalty specification of the versatile link systems 

D. Gong, ${ }^{a}$ C. Liu, ${ }^{a}$ T. Liu, ${ }^{a}$ T. Huffman, ${ }^{b}$ A. Prosser, ${ }^{c}$ J. Troska, ${ }^{d}$ F. Vasey, ${ }^{d}$<br>A. Weidberg, ${ }^{b}$ A. Xiang, ${ }^{a, 1}$ J. Ye ${ }^{a}$ and L. Zhu ${ }^{a}$<br>${ }^{a}$ Southern Methodist University, Department of Physics, Dallas, Texas, U.S.A.<br>${ }^{b}$ Oxford University, Department of Physics, Oxford, U.K.<br>${ }^{c}$ Fermilab, Electronic Systems Engineering (ESE) Department, Batavia, Illinois, U.S.A.<br>${ }^{d}$ CERN, Physics and Engineering Department, Geneva, Switzerland<br>E-mail: cxiang@smu.edu<br>AbSTRACT: This paper presents simulation and experimental studies of optical power penalties on the Versatile Link, a common R\&D project on high-speed optical link for SLHC experiments. The 10 Gigabit Ethernet (10GbE) link model is examined and conservative link power penalties are predicted. We conduct parameter sensitivity analyses and find that the transmitter characteristics affect the link power penalties most. Power penalty differences of multi-mode and single-mode commerical transceiver modules over different fiber lengths are tested to be within the simulation limits. The optical power budgets are then proposed for different Versatile Link variants.

Keywords: Optical detector readout concepts; Radiation-hard electronics; Front-end electronics for detector readout

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## 1 Introducion

The Versatile Link project aims to provide a radiation and magnetic field tolerant, high-speed (4.8 Gbps tentative) optical link for the readout and control of SLHC experiments [1]. For a large scale integration project like this, a system level specification is required to ensure the functionality, environmental resistance and operational reliability of the Versatile Link in the proposed applications. One of the most important metrics to be determined is the optical power budget, which specifies a link's signal strengths and power allocations for a given level of performance. On one hand, the distribution of the available power among the link segments should take into account the full range of transmission penalties, the radiation induced degradations as well as a safety margin for unexpected losses. On the other hand, the required optical power levels of the link transceivers should not exceed the manufacturability of these components.

Relevant industrial standards are 10GBASE-SR and 10GBASE-LR as well as fiber channel 400-SM-LC and 400-M5E-SN [2, 3], which have gained international support over the years and to which the commercial components, namely, the back-end, of the Versatile Link will comply. Due to the design philosophy of "worst case" operations and the "interoperability" use of components, optical power budget recommendations by these standards are quite conservative and leave no margins for customization. Since the Versatile Link operates at a lower data rate and a shorter target length (around 150 meters from the front-end detector to the back-end counting room), it is beneficial to re-evaluate the link penalties. More importantly, since the Versatile Link frontend components are expected to suffer significant power degradation from radiation during their lifetimes, and the total losses cannot be accommodated by the existing margins, it is necessary to re-examine the power level limits on the link components. The goal is to propose a conservative yet realistic power budget.

In section 2, the typical Versatile Link transmission scheme and the optical link budget process are described. The IEEE 10GbE link model is investigated in section 3, where bit error rate (BER)


Figure 1. Block diagram of a possible data transmission scheme using the Versatile Link.
measurements on reference links with commercial transceivers are also reported. A crucial part of the power budget is based on the knowledge of device radiation tolerance. This is discussed in section 4. The overall Versatile Link power budget is proposed in section 5 followed by a concluding discussion in section 6 .

## 2 Optical link power budget

The physical layer of a typical optical link comprises the laser-based transmitter circuitry, the PIN photodiode-based receiver circuitry and the fiber medium. A block diagram of a possible transmission scheme deployed by the Versatile Link is shown in figure 1. The central red block encompasses the Versatile Link components. The link is bi-directional and accommodates devices that support both multi-mode operation with a center-wavelength of 850 nm and single-mode operation with a center-wavelength of 1310 nm .

Two types of electro-optical transceivers are used in the Versatile Link. The on detector module, the versatile transceiver (VTRx), will be custom designed. It consists of a radiation tolerant laser driver (LDD) and a qualified laser diode on the transmitting side; a qualified PIN diode and a radiation tolerant post-amplifier (TIA) on the receiving side. The off detector module, the standard transceiver (TRx), will be procured commercial-off-the-shelf (COTS), as will be the fiber cables.

Given the on and off detector transceiver differences and the two wavelengths of operation, four link variants are specified individually. In the MM_VTx_Rx and the SM_VTx_Rx configurations, data flow from the versatile transmitter on detectors to a standard receiver in the counting room, using multi-mode and single-mode transceiver modules and over multi-mode and singlemode fibers, respectively. In the MM_Tx_VRx and the SM_Tx_VRx configurations, data flow in the opposite direction from standard transmitters in the counting room to the versatile receivers on detector.

To ensure a link BER below $10^{-12}$ at the target data rate and fiber length, across operation temperatures and throughout life cycle, the optical power budget must be carefully planned ahead so that an adequate receiving signal-to-noise ratio is maintained under all conditions. The process is mapped as the allocation of available power among various loss components, as shown in figure 2. The amount of optical power launched into the link is deduced from the difference between the transmitter minimum output, i.e., Tx_OMA_min (OMA - optical modulation am-


Figure 2. Power budget process in an optical link.

Table 1. Key characteristics in support of the Versatile Link model simulation.

|  | MM_VL | SM VL |
| :--- | :---: | :---: |
| Data rate (Gbps) | 5 | 5 |
| Link length (meter) | 150 | 150 |
| Center wavelength (nm) | 850 | 1310 |
| RMS spectral width (nm) | 0.49 | 0.2 |
| Optical rise/fall time (ps) | 75 | 75 |
| Relative intensity noise (dB/Hz) | -130 | -130 |
| Mode partition noise coefficient | 0.3 | 0 |
| Reflection coefficient | 0 | 0.6 |

plitude) and the receiver minimum power input, i.e. Rx_sensitivity_OMA. The proposed Versatile Link transceiver power levels are discussed in section 5. Link penalties arising from various mechanisms are discussed in section 3. Since the Versatile Link is designed to meet the requirements of SLHC experiments, allowance must be allocated to radiation degradations, as are described in section 4 . Finally, engineering judgment is called for in the assignment of a safety margin.

## 3 Link model and BER test

An open source 10 GbE link model has been developed by the IEEE high speed working group as a tool to facilitate optical physical layer specifications. The model calculates impairments caused by inter-symbol-interference (ISI), mode partition noise (MPN), relative intensity noise (RIN), duty-cycle-distortion (DCD), etc. These nonlinear effects result in an increased aggregated link power penalty as the data rate and link length increase.

The link model is populated with key parameter values that represent the Versatile Link operation conditions, as summarized in table 1 . The simulation renders a maximum penalty of 1.0 dB for the multi-mode versatile link and a maximum penalty of 1.5 dB for the single-mode versatile link operations. Compared to 4.7 dB and 3.2 dB in the 10GBASE-S and 10GBASE-L budgets, the allocation for link penalties are largely reduced since the Versatile Link operates at a lower data rate and shorter reach.

Power penalty dependence on the transmitter, fiber and receiver characteristics was examined and two sets of sensitivity charts are shown in figure 3 . We found that in the multi-mode link, power penalty is most sensitive to the optical rise/fall time, $\mathrm{T}_{r / f}(20 \%-80 \%)$, in the sense that the power penalty change is steep in a wide working range. Whereas for the other parameters, i.e., RIN noise, RMS spectral width and receiver bandwidth, the power penalty change is relatively flat in certain working ranges. In the single-mode link, reflection is another sensitive parameter. But the reflection can be controlled through isolators or angle polished connectors to be less than -12 dB .


Figure 3. Top: MM_VL link and bottom: SM_VL link characteristic sensitivity charts.


Figure 4. Link power penalties deduced from BER measurements. Left: differences among multi-mode links; right: differences among single-mode links (OMA - optical modulation amplitude measured at the receiver input).

In the previous table, the optical rise/fall time is set to the high end of the target working range to ensure the conservativeness of the link analyzed.

Measurement of link power penalty requires comparison of BER over a typical range since the power penalty is manifested as the horizontal shift in the BER curves. Both multi-mode and single-mode links are constructed using a batch of commercial transceiver modules. A number of different transmitters are launched into different fibers and connected to one reference receiver. The fibers range from 2 meters to 150 meters. Figure 4 shows that power penalty differences among these links are all below 1.5 dB . It further shows that the performance variations of the transmitters have a slightly larger impact on power penalties than the performance and length variations of the fibers at this range. The link model predictions correlate well with these experimental results and are hence adapted in the power budget calculations presented in section 5 .

## 4 Radiation degradation

Qualified Versatile Link front-end components must withstand a level of radiation up to the SLHC level. In addition, their radiation induced power degradation must fit in the allowance allocated in the overall link budget. Candidate laser, PIN, driver, amplifier and fibers are examined in [5, 6].

Table 2. Versatile Link power budget table with 4 variants.

| configuration/parameter | MM_VTx_Rx | $M_{M}$ _Tx_VRx | SM_VTx_Rx | SM_Tx_VRx |
| :--- | :---: | :---: | :---: | :---: |
| Transceiverpower level |  |  |  |  |
| Tx OMA min | -3.8 dBm | -2.0 dBm | -3.2 dBm | -2.8 dBm |
| Rx Sensitivity OMA | -11.1 dBm | -13.1 dBm | -12.6 dBm | -15.4 dBm |
| Power budget (Tx - Rx) | 7.3 dB | 7.3 dB | 9.4 dB | 9.4 dB |
| Fiber attenuation | 0.6 dB | 0.6 dB | 0.1 dB | 0.1 dB |
| Connection and splice loss | 1.5 dB | 1.5 dB | 2.0 dB | 2.0 dB |
| Link penalties | 1.0 dB | 1.0 dB | 1.5 dB | 1.5 dB |
| Tx irradiation degradation | - | - | - | - |
| Rx irradiation degradation | - | 7.0 dB | - | 9.0 dB |
| Fiber irradiation degradation | 1.0 dB | 1.0 dB | - | - |
| Margin | 3.2 dB | 0.0 dB | 5.8 dB | 0.0 dB |

Sources of degradations are described below. Tested or extrapolated to a maximum exposed radiation of $6 \times 10^{15} \mathrm{~cm}^{-2}$ neutron fluence, the corresponding degradation allowances are also allocated.

Both the vertical cavity surface emitting (VCSEL) based multi-mode lasers and the FabryPerot (FP) based single-mode lasers show increased threshold current and decreased slope efficiency. Yet the transmitter power loss should be compensated by increasing drive current and should not exceed 0.05 dB . Both GaAs based multi-mode PIN diodes and InGaAs based singlemode PIN diodes show decreased responsivity, while the InGaAs PIN diodes also suffer from increased leakage current. Overall receiver sensitivity degradations should not exceed 9.6 dB for GaAs devices and 5.4 dB for InGaAs devices. PIN diode and post amplifier circuits are also vulnerable to single event upsets (SEU). A customized coding scheme successfully demonstrated the resistance against SEU induced single and burst errors. Different fiber types degrade differently. Radiation induced attenuation is worse at cold temperatures. A few radiation resistant grade candidates are identified and expected to perform most optimistically. Qualified fiber radiation induced attenuation should not exceed 1.0 dB for multi-mode fibers and 0.05 dB for single-mode fibers.

## 5 Power penalty specification

Power budget specifications are then proposed for the four variants of the Versatile Link, as listed in table 2. In addition to link penalties and radiation degradations described in the previous sections, fiber attenuation is $3.5 \mathrm{~dB} / \mathrm{km}$ for multi-mode and $0.4 \mathrm{~dB} / \mathrm{km}$ for single-mode. Connector and splice loss is 1.5 dB for multi-mode and 2.0 dB for single-mode, which supports 3 or 4 connections with an insertion loss of no more than 0.5 dB each.

Standard 10GbE compliant transmitter power and receiver sensitivity specifications are applied to the two uplinks, MM_VTx_Rx and SM_VTx_Rx. After the modification on link penalties and the insertion of radiation degradations, these two uplinks meet budget with an increased safety margin. In the two downlinks, MM_Tx_VRx and SM_Tx_VRx, the specifications of the versatile receiver and the corresponding transmitter must exceed those of the standard modules in order to compensate for the large radiation deficits. These elevated power requirements on the downlink transceivers are within technology limits, but mandate individual screening tests. And the safety margin is reduced to zero.

## 6 Conclusion

Link model simulations and BER tests are performed to evaluate the optical power penalties in the Versatile Link power budget. The results conform well and support a sizable reduction in the allocation for link penalties. However, to accommodate the radiation degradation of the front-end components, power levels of the downlink transceivers still need to be elevated.

Currently there are not enough safety margins to cover environmental and other unexpected losses in the down links. Several further explorations are possible. At the system level, receiver degradation can be relieved by positioning the components further away from detector. At the component level, extra power can be garnered by modest redesign of the laser coupling interface. At the data transmission level, custom coding is known to provide single event upset resistance, which can be quantified as potential power gain.

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Response of a $0.25 \mu \mathrm{~m}$ thin-film silicon-on-sapphire CMOS technology to total ionizing dose

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# Response of a $0.25 \mu \mathrm{~m}$ thin-film silicon-on-sapphire CMOS technology to total ionizing dose 

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ABSTRACT: The radiation response of a $0.25 \mu \mathrm{~m}$ silicon-on-sapphire CMOS technology is characterized at the transistor and circuit levels utilizing both standard and enclosed layout devices. The threshold-voltage shift is less than 170 mV and the leakage-current increase is less than 1 nA for individual standard-layout nMOSFET and pMOSFET devices at a total dose of $100 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$. The increase in power supply current at the circuit level was less than $5 \%$, consistent with the small change in off-state transistor leakage current. The technology exhibits good characteristics for use in the electronics of the ATLAS experiment at the Large Hadron Collider.

KEYWORDS: Radiation damage to electronic components; Radiation-hard electronics

[^51]
## Contents

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2 Test structures and experimental conditions ..... 1
3 Experimental results ..... 2
4 Conclusions ..... 4

## 1 Introduction

Silicon-on-sapphire (SoS) complementary metal-oxide-semiconductor (CMOS) technology has been used in radiation-tolerant applications since the 1970s. SoS technologies exhibit several characteristics that make them attractive for use in radiation environments, including an insulating sapphire layer below the active silicon that eliminates the parasitic inter-device bipolar structure associated with latchup in bulk devices. SoS technologies also have been reported to have smaller singleevent upset cross-sections than equivalent bulk processes [1]. However, radiation-induced leakage currents along the edges of the device and the back channel, where the active silicon meets the sapphire substrate, are important issues in these technologies [2]. The ATLAS experiment at the Large Hadron Collider is one example of an application for which SoS technology is very promising; the radiation environment is quite challenging compared to typical space and defense applications [3].

In this work, the radiation response of a $0.25 \mu \mathrm{~m}$ SoS CMOS technology is characterized at the transistor and circuit levels. Devices are evaluated in both standard and enclosed layout geometries. Radiation-induced charge trapping in the gate oxide results in threshold voltage shifts less than 170 mV for standard-layout transistors irradiated to a total dose of $100 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$. Additionally, increases in radiation-induced leakage current are less than 1 nA for standard-layout nMOSFET and pMOSFET devices. Circuit-level evaluation of these structures is consistent with these results.

## 2 Test structures and experimental conditions

The Peregrine $0.25 \mu \mathrm{~m}$ SoS process is a thin-film technology with both partially depleted and fully depleted devices. The epitaxial silicon layer is 80 nm thick with a $200 \mu \mathrm{~m}$ sapphire insulating substrate. The gate oxide thickness is 6 nm , and the process uses LOCOS for device isolation. Individual transistors and a set of shift registers were fabricated on a test chip.

Structures were fabricated in either standard or enclosed layout geometries. Three different transistor types were used with high, regular, or intrinsic threshold voltages. Devices with regular and high threshold voltages are partially depleted, while the intrinsic devices are fully depleted. Devices were packaged and subsequently baked for twelve hours at $150^{\circ} \mathrm{C}$ in preparation for irradiation. nMOSFET and pMOSFET irradiation bias conditions were $V_{D}=2.5 \mathrm{~V}$ and -2.5 V ,


Figure 1. $I_{D}-V_{G}$ characteristics of an enclosed layout; regular threshold voltage nMOS SOS transistor.


Figure 2. $I_{D}-V_{G}$ characteristics of an enclosed layout; regular threshold voltage pMOS SOS transistor.
respectively; all other terminals were grounded. This off-state condition is the worst case for inverters exposed to total ionizing dose [4]. The transistors were irradiated with 10 keV x -rays at a dose rate of $31.5 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$ per minute using an ARACOR Model 4100 irradiator. $I_{D}-V_{G}$ sweeps were performed to characterize the leakage current and threshold voltage of irradiated devices. Device characterization was performed with an HP 4156A parameter analyzer with an applied drain bias of $\pm 0.1 \mathrm{~V}$ for nMOS and pMOS transistors, respectively. Gate voltages were swept between -1.5 V and 1.5 V . The source and sapphire substrate were grounded during device characterization and irradiation.

Two types of shift registers, consisting of 32 D-flip-flop stages, one using standard layout transistors, the other enclosed layout transistors, were fabricated for circuit-level evaluation of radiation-induced leakage current. The power supply voltage for the shift registers was 2.5 V with the substrate grounded. The shift registers were irradiated with 198 MeV protons to a total fluence of $1.27 \times 10^{13} \mathrm{~cm}^{-2}$ [5]. The operating frequency during irradiation was 40 MHz ; the power supply current for each shift register was monitored with a Keithley 2700 multi-channel digital multimeter.

## 3 Experimental results

Typical pre- and post-irradiation $I_{D}-V_{G}$ characteristics are shown in figures 1 and 2 for nMOS and pMOS transistors. These devices are enclosed layout, regular threshold voltage devices, corresponding to $V_{T}=0.55 \mathrm{~V}$ and -0.35 V , for nMOS and pMOS transistors, respectively.

An initial positive shift in threshold voltage, with a maximum value of 170 mV , was observed at less than $1 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$ in both nMOSFET and pMOSFET devices, as seen in figure 3. This initial shift is due to radiation-induced electron trapping in the sapphire substrate [6]. These trapped electrons accumulate the back channel of nMOSFETs, and the front to back coupling results in a shift in threshold voltage. In pMOSFETs the trapped electrons couple the front and back gate similarly; however, they deplete the n-type body, leading to additional leakage current. No additional threshold-voltage shifts were observed following the initial exposure of $10 \operatorname{krad}\left(\mathrm{SiO}_{2}\right)$, up to the largest dose considered here ( $100 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$ ).


Figure 3. $\Delta V_{T}$ as a function of dose for partially depleted nMOS and pMOS devices.


Figure 4. Change in leakage current with dose for high and regular threshold pMOSFETs with standard and enclosed layouts.


Figure 5. Change in leakage current with dose for high and regular threshold nMOSFETs with standard and enclosed layouts.

The radiation-induced leakage currents for standard and enclosed layout devices are shown in figures 4 and 5 for pMOSFETs and nMOSFETs, respectively. nMOS transistors in a standard layout configuration exhibit a parasitic conductive path along the edge of the device [7]. The enclosed layout transistors eliminate the edge leakage paths present in the standard layout nMOS devices. The edge leakage is associated with hole trapping in the isolation oxide, which affects nMOS transistors. Conversely, leakage paths exist for pMOS transistors primarily along the back channel of the device due to electron trapping, which impacts the threshold voltage of both nMOS and pMOS transistors. This back-channel leakage path exists and impacts both standard and enclosed layout device geometries.

The post-irradiation increase in power supply current at the circuit level is less than $5 \%$ (see figure 6), which is consistent with the relatively small radiation-induced change in off-state transistor leakage (less than 1 nA at $100 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$ for both nMOSFET and pMOSFET devices). Leakage current was consistently higher for standard-layout devices than for enclosed-layout devices following irradiation because of the elimination of the parasitic edge leakage path in the enclosedlayout devices. The increase in circuit-level leakage current with increasing dose is caused by the formation of a back channel in the pMOS devices along the sapphire-silicon interface.


Figure 6. Normalized power supply current of standard and enclosed layout shift registers irradiated with 198 MeV protons.

## 4 Conclusions

Single transistors and shift registers fabricated in a $0.25 \mu \mathrm{~m}$ SoS CMOS technology were irradiated with 10 keV x-rays and 198 MeV protons, respectively. Radiation-induced electron trapping at the silicon-sapphire interface results in a shift in threshold voltage for both nMOS and pMOS transistors. The magnitude of the threshold-voltage shift was less than 170 mV , and saturated within $1 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$. At the transistor level, standard-layout pMOSFETs exhibited the largest increases in leakage current due to electron trapping at the back-channel interface. Radiation-induced leakage current was 1 nA or less for all device variants. This result is consistent with circuit-level results during proton irradiation of shift registers, and had little impact on circuit operation. These results indicate that this $0.25 \mu \mathrm{~m}$ SoS technology exhibits stable operating characteristics in a total dose environment of $100 \mathrm{krad}\left(\mathrm{SiO}_{2}\right)$, and appears to be very well suited for operating in the ATLAS TID environment.

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#### Abstract

Optical fibers in the readout system for the Large Hadron Collider (LHC) upgrades will operate in a harsh radiactive environment. The fibers within 12 meters from the front-end detectors are exposed up to total ionizing dose of $250 \mathrm{kGy}(\mathrm{Si})$ in their 10 year operational lifetime. In some applications, the fibers within the tracking volume are kept in a cold environment near $-25^{\circ} \mathrm{C}$. The paper presents the identification of suitable optical fibers for the LHC detector upgrades. Several optical fibers have been tested to $650 \mathrm{kGy}(\mathrm{Si})$ at room temperature with various dose rates of 60Co gamma rays. Two multi-mode fibers and one single-mode fiber have been qualified for use in the LHC upgrades for warm operations. Four optical fibers have been tested to $500 \mathrm{kGy}(\mathrm{Si})$ at $-25^{\circ} \mathrm{C}$ with $27 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr} 60 \mathrm{Co}$ gamma rays. Two SM fibers have been qualified for the LHC upgrades for cold operations. Several optical fibers, including two MM fibers, have been tested up to $11 \mathrm{kGy}(\mathrm{Si})$ at $-25^{\circ} \mathrm{C}$ with $70 \mathrm{~Gy}(\mathrm{Si}) / \mathrm{hr} 60 \mathrm{Co}$ gamma rays and exhibited moderate radiation induced attenuation (RIA, indicating that all tested fibers are potential candidates for the LHC upgrades for warm and cold operations.


Response to Reviewers: Reviewers' comments:
"Reviewer \#1: I think the manuscript is almost okay for the publication. But I have still a few questions and comments. I am happy if the authors think my comments and revise slightly the manuscript.

1. Figure 1(a),(b) and (c): I don't think readers will get so much information from the figures. The context can be understood without these figures actually. It may be better not to shown. I don't think the photographs are essential for the interpretation of data taken in BNL (Fig.5). But this is just my comment and to follow or ignore my idea is up to you.
2. In Page 5, a formula of RIA depicted in 3 Experimental Results must be rewritten: RIA $=10$ *log_10... should be RIA=10log_10... or $10 \times \log \_10 \ldots$ Usually "*" does not mean the multiplication operator.
3. Please discuss why you set threshold as about $0.1 \mathrm{~dB} / \mathrm{m}$ for robust fibers to be used in the future LHC experiment.
4. Please discuss how much dose rate is expected in the actual LHC experiment. I don't think there is an explicit value written in the paper. If you cannot evaluate the value precisely, then give just (even rough) range of expectation (In Page 10 Line 7)." [Numbering mine.]

Response to Reviewer Comment No. 1: I decided to keep these figures, as they provide a visual representation of the experiment setups. Also, Figure 1(a) in particular is very helpful for understanding the cooling system used at SCK-CEN.

Response to Reviewer Comment No. 2: The * symbol in the RIA formula was replaced with a x symbol.
Response to Reviewer Comment No. 3: To my knowledge, the paper does not explicitly mention a 0.1 $\mathrm{dB} / \mathrm{m}$ threshold; figures with this $\mathrm{dB} / \mathrm{m}$ unit only appear in discussions of the results. However, I did add the following sentence to paragraph 4 of the introduction (page 2), "The total RIA should not exceed 1.0 dB for MM fibers or 0.05 dB for SM fibers; these limits are set by the power budget of the link system [6]."

Response to Reviewer Comment No. 4: The paper does provide estimates of the actual LHC total dose and dose rate. An estimated total dose of 250 kGy is mentioned in the abstract and in paragraph 3 of the introduction (page 2), and an estimated dose rate of $9 \mathrm{~Gy} / \mathrm{hr}$ is given in paragraph 1 of page 7 . I reiterated this dose rate estimate in the conclusion.

TIPP 2011 - Technology and Instrumentation in Particle Physics 2011

# The radiation tolerance of specific optical fibers for the LHC upgrades 

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#### Abstract

Optical fibers in the readout system for the Large Hadron Collider (LHC) upgrades will operate in a harsh radiactive environment. The fibers within 12 meters from the front-end detectors are exposed up to total ionizing dose of 250 $\mathrm{kGy}(\mathrm{Si})$ in their 10 year operational lifetime. In some applications, the fibers within the tracking volume are kept in a cold environment near $-25^{\circ} \mathrm{C}$. The paper presents the identification of suitable optical fibers for the LHC detector upgrades. Several optical fibers have been tested to $650 \mathrm{kGy}(\mathrm{Si})$ at room temperature with various dose rates of ${ }^{60} \mathrm{Co}$ gamma rays. Two multi-mode fibers and one single-mode fiber have been qualified for use in the LHC upgrades for warm operations. Four optical fibers have been tested to $500 \mathrm{kGy}(\mathrm{Si})$ at $-25^{\circ} \mathrm{C}$ with $27 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr} 60 \mathrm{Co}$ gamma rays. Two SM fibers have been qualified for the LHC upgrades for cold operations. Several optical fibers, including two MM fibers, have been tested up to $11 \mathrm{kGy}(\mathrm{Si})$ at $-25^{\circ} \mathrm{C}$ with $70 \mathrm{~Gy}(\mathrm{Si}) / \mathrm{hr}{ }^{60} \mathrm{Co}$ gamma rays and exhibited moderate radiation induced attenuation (RIA, indicating that all tested fibers are potential candidates for the LHC upgrades for warm and cold operations.


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Keywords: Radiation damage to electronic components; Radiation damage evaluation methods; Optical detector readout concepts

[^52]
## 1. Introduction

Optical fibers are materials with a high refractive index used to transmit data in the form of light over long distances. Utilizing dielectric wave guide techniques, optical fibers allow for such data transmission to occur with a negligible loss of signal strength. They most commonly consist of a silica glass core surrounded with cladding of a slightly different refractive index; this construction induces total internal reflection. Light propagates through optical fibers with little attenuation, and the signal can be modulated at a very high rate. The two main categories of optical fiber are multi-mode (MM) and single-mode (SM). MM fibers have a larger core diameter and support many propagation paths or transverse modes. They are generally used for short-distance communication links. SM fibers have a much smaller core diameter, usually less than ten times the propagating wavelength, and support only one transverse mode. They are typically used for longer links. To meet the detector data transmission objectives, both MM and SM systems have been proposed [1].

The ATLAS [2] (A Toroidal LHC Apparatus) and CMS [3] (Compact Muon Solenoid) particle physics experiments at the European Organization for Nuclear Research (CERN) seek to learn about the forces that formed and still act on the universe. Using the Large Hadron Collider (LHC), scientists from all over the world monitor collisions of high-energy particles that replicate the state of the universe at its very beginnings. Detection systems identify the particles involved and record their energy and momentum. Amongst other objectives, ATLAS and CMS seek to discover the Higgs boson, extra dimensions, and dark matter.

Both the ATLAS and CMS experiments use optical fibers to transfer data between front-end detectors and back-end computers. The fibers within 12 meters of the front-end detectors are exposed to a total ionizing dose of up to $250 \mathrm{kGy}(\mathrm{Si})$ in their 10 -year operational lifetime [4]. In some applications, the 2 meters closest to the front end are kept in a cold environment near $-25^{\circ} \mathrm{C}$. Ionizing radiation damages the molecular structure of the fibers' glass cores, creating charged scattering sites. These sites cause the light transmitted down the fiber to scatter into non-propagating modes, resulting in radiation-induced absorption (RIA) along the length of the fiber [4]. The fibers within the ATLAS and CMS detectors would need to maintain a pre-qualified attenuation while withstanding high radiation doses and low temperatures.

The Versatile Link Project was founded in April 2008 to develop a radiation-tolerant optical interface for the proposed LHC upgrades. This interface requires bidirectional data transmission capabilities of up to $5 \mathrm{~Gb} / \mathrm{s}$ via optical fibers that are qualified to withstand radiation doses of up to $500 \mathrm{kGy}(\mathrm{Si})$ at room temperature and at low temperatures of approximately $-25^{\circ} \mathrm{C}$ [5]. The upgrade is to utilize either MM fibers with an operational wavelength of 850 nm or SM fibers with an operational wavelength of 1310 nm . The total RIA should not exceed 1.0 dB for MM fibers or 0.05 dB for SM fibers; these limits are set by the power budget of the link system [6]. The total RIA should be calculated via a worst-case piecewise fiber routing. Scientists from CERN, Oxford University, Fermi National Laboratory, and Southern Methodist University (SMU) work on the project.

## 2. Experimental Setup

As an important step towards achieving its goals, the Versatile Link Project is testing off-the-shelf optical fibers for radiation tolerance. As of TIPP 2011, four experiments have been conducted, subjecting the fibers to various radiation doses at either room temperature or at approximately $-25^{\circ} \mathrm{C}$. Table 1 lists the fibers that have been tested thus far. The Corning fibers were commercially available as of the tests described in this paper, although the Infinicor SX+ can no longer be purchased. None of the Draka fibers tested reached the open market, but instead served as prototypes for the DrakaElite ${ }^{\text {TM }}$ line of MM and SM
fibers. Some of these fibers will be tested in the future. Fibres X and Y are patent-pending designs produced by CERN and undisclosed companies.

Table 1. Fibers tested

| Manufacturer | Part number | MM/SM | Operational wavelength (nm) |
| :---: | :---: | :---: | :---: |
| Corning [7] | ClearCurve OM3 | MM | 850 |
|  | Infinicor SX+ | MM | 850 |
|  | SMF-28 | SM | 1310 |
|  | SMF-28e+ | SM | 1310 |
|  | SMF-28XB | SM | 1310 |
| Draka [8] | Draka-1 | MM | 850 |
|  | RHP-1 | MM | 850 |
|  | RHP-1 SRH | MM | 850 |
|  | RHP-2 | MM | 850 |
| Manufacturer X | Fibre X | SM | 1310 |
| Manufacturer Y | Fibre Y | SM | 1310 |

The Belgian Nuclear Research Center (SCK-CEN) near Mol, Belgium is one of two facilities at which the Versatile Link Project has carried out its fiber radiation tests. Two gamma radiation sources at SCKCEN bombarded the fibers to simulate the LHC's radioactive environment. The "Brigitte" source utilized rods of ${ }^{60} \mathrm{Co}$ to deliver high dose rates of up to $27 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$. The "Rita" source, also ${ }^{60} \mathrm{Co}$, provided dose rates of up to $1.01 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$. As a side note, gamma radiation sources were chosen for safety reasons; once the sources were covered, the radiation dissipated within seconds.

No temperature control system was used for the experiments conducted at room temperature. For the tests conducted at $-25^{\circ} \mathrm{C}$, however, a dual-phase temperature control system was developed at Oxford for use at SCK-CEN. Carbon dioxide $\left(\mathrm{CO}_{2}\right)$ entered the system at a pressure of 50 bar and condensed into a liquid via the Joule-Kelvin Effect; the work done by high-pressure $\mathrm{CO}_{2}$ to overcome the impedance of very narrow capillary tubes caused the temperature to decrease. The fibers were then cooled as $\mathrm{CO}_{2}$ evaporated in liquid-gas dual-phase. A Back Pressure Regulator regulated the dual-phase system's pressure, which in turn allowed the fibers' temperature to be controlled. After cooling the fibers, the cold, low pressure $\mathrm{CO}_{2}$ was also used to cool the incoming high pressure gas in a double-pipe heat exchanger; this last process increased the system's efficiency [9]. Figure 1(a) provides a graphical representation of this cooling system.

The other fiber testing site was Brookhaven National Laboratory (BNL) in Upton, New York. A ${ }^{60} \mathrm{Co}$ gamma source, housed within a cylindrical containment vessel, provided a dose rate of up to 0.4 $\mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$ at a 20 cm by 20 cm window in the source container. The dose rate was adjusted by placing the fibers at different distances from the source; higher doses could be obtained by placing a sample inside the window. Figure 1(b) illustrates this setup. For the low temperature experiments, the fibers were placed in a chest freezer in order to keep them at an ambient temperature of $-25^{\circ} \mathrm{C}$ [10]. The freezer's control electronics were shielded with lead bricks so that they would not be damaged by radiation. The fibers were routed into the freezer and coiled within the path of the radiation. Figure 1(c) shows the freezer's interior.


Fig. 1. (a) Schematic diagram of SCK-CEN's $\mathrm{CO}_{2}$ cooling system


Fig. 1. (b) Radiation source containment vessel (left) and chest freezer (right) used for fiber tests at BNL


Fig. 1. (c) Inside of chest freezer at BNL

## 3. Experimental Results

To evaluate the effectiveness of each fiber under radiation, a signal was propagated at one end and then measured at the other. Vertical Cavity Surface-Emitting Lasers (VCSEL's) channelled light of a 850 nm wavelength through the MM fibers, while Edge-Emitting Lasers (EEL's) directed light of a $1,310 \mathrm{~nm}$ wavelength through the SM fibers. At the end of each fiber opposite the light source, the remaining signal was converted to a voltage and measured. Each voltage was then translated into optical power, and each power result was used in Equation 1, where $P(t)$ is optical power at time $t$ and $t_{0}$ is the time the irradiation started, to determine the fiber's radiation-induced attenuation (RIA) at its particular time.

$$
\begin{equation*}
R I A=10 \times \log _{10}\left[\frac{P_{t_{0}}}{P t}\right] \tag{1}
\end{equation*}
$$

Figure 2 depicts the results of an experiment conducted in 2008 at the SCK-CEN "Brigitte" and BNL facilities. When tested to a total dose of $650 \mathrm{kGy}(\mathrm{Si})$ at a dose rate of $22.5 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$, all of the MM fibers tested (the Infinicor SX+, Draka-1, Draka-RHP-1, and Draka RHP-2) performed reasonably well. The RIA that they experienced was between 0.1 and $0.5 \mathrm{~dB} / \mathrm{m}$ [4]. The Infinicor SX+ was also tested at BNL to a total dose of $10 \mathrm{kGy}(\mathrm{Si})$, at dose rates of $0.424,0.343$, and $0.0265 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$; peak RIA was $0.06 \mathrm{~dB} / \mathrm{m}$ in these conditions [4]. Of the fibers tested, only the Infinicor SX+ and Draka-RHP-1 were judged sufficiently robust to be qualified for warm operations at the LHC. The only SM fiber tested, the Corning SMF-28, was a standout performer; its peak RIA was less than $0.07 \mathrm{~dB} / \mathrm{m}$ when tested to 650 $\mathrm{kGy}(\mathrm{Si})$ at $22.5 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}[4]$.


Fig. 2. (a) Results at room temperature under a dose rate of $22.5 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$ for Draka-1 (green), Draka-RHP-2 (blue), Infinicor SX+ (red), and Draka-RHP-1 (black); SCK-CEN


Fig. 2. (b) SM results at room-temperature; SCK-CEN

An interesting result of the high-dose experiments was an early attenuation spike, which was followed by a less rapid decrease in RIA and then another increase. The reason for the pattern is not clear, but it is probably due to two different damage processes. The high initial attenuation is due to the incoming radiation filling naturally-occurring defects within the fibers, known as Self-Trapped Holes (STH). In a high dose environment, these holes fill within minutes of exposure to radiation, bringing RIA to a maximum. At the same time, the corresponding annealing process works to break the STH bonds, eventually causing the attenuation to fall. This latter process is dependent on both the nature of the fiber and the ambient temperature. For the high dose experiments depicted in Figure 2, the fibers were constrained by three solid aluminium disks, each 220 mm in diameter and 10 mm in thickness. The high energy gamma ray photons resulting from ${ }^{60} \mathrm{Co}$ decay Compton scattered off the aluminium's electrons. Since the gamma rays were of high enough energy, the Compton scattering produced measurable heat. At the start of the RIA decline for each of the fibers, temperature had increased by $5^{\circ} \mathrm{C}$; it possible that this rise in temperature spurred the annealing process to a higher rate than the attenuation. The other damage process is the newly induced radiation damage to the fiber's core. This process eventually took over in the high dose experiments, after the temperature stabilized and the STH annealing ended. The annealing of newly induced radiation damage had little effect, as evidenced by the consistent increase in RIA until the end of the experiment [4]. Continued monitoring of the fibers after the tests, though, revealed that RIA decreased over time after irradiation. Ultimately, these processes are still not well understood. However, the Versatile Link Project is concerned with dose rates on the order of $9 \mathrm{~Gy}(\mathrm{Si}) / \mathrm{hr}$, calculated by dividing the estimated 250 kGy total dose by $10^{8}$ seconds of operation over the course of 10 years. Since the STH effect only occurs at high dose rates, it was ignored in the route specific RIA calculations.

Figure 3 depicts the results of an experiment conducted in 2009 at the SCK-CEN "Rita" facility. The Draka-RHP-1 fiber was tested to a total dose of $30 \mathrm{kGy}(\mathrm{Si})$ at a dose rate of $0.5 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$, at temperatures of -4 and $-25.5^{\circ} \mathrm{C}$. This experiment was the first in which the RIA of candidate fibers was studied near the operating temperature of optical fibers in the ATLAS and CMS experiments. The maximum RIA was $\sim 0.05 \mathrm{~dB} / \mathrm{m}$; the fiber experienced this RIA at the lower temperature of $-25.5^{\circ} \mathrm{C}$ [11]. This temperature dependence is a result of the ambient temperature's effect on the annealing process. At lower temperatures the rate of annealing is significantly reduced, resulting in a higher RIA.


Fig. 3. RIA of Draka-RHP-1 at -4 (red) and -25 (blue) ${ }^{\circ} \mathrm{C}$

Figure 4 depicts the results of an experiment conducted in 2010 at the SCK-CEN "Brigitte" facility, in which several fibers were tested at $-25^{\circ} \mathrm{C}$ and $27 \mathrm{kGy}(\mathrm{Si}) / \mathrm{hr}$ to $500 \mathrm{kGy}(\mathrm{Si})$, approximately twice the total lifetime dose the fibers would experience in operation at the LHC. Two of the SM fibers tested, Fibres X and Y, experienced very low RIA and, as such, were qualified for use at the LHC. The other SM fiber, the SMF-28e+, and the one MM fiber tested, the Infinicor SX+, saturated almost immediately; the RIA for both of these fibers fluctuated between $\sim 1 \mathrm{~dB} / \mathrm{m}$, the maximum possible value, and $\sim 0.8 \mathrm{~dB} / \mathrm{m}$ [11]. If such an RIA were to occur in service at the LHC, the fibers would be rendered inoperative. However, because of the experiment's very high dose rate, the Infinicor and SMF-28e+ cannot necessarily be excluded as candidates for the LHC upgrades.


Fig. 4. (a) RIA of Fibre Y


Fig. 4. (b) RIA of Fibre X


Fig. 4. (c) RIA of Infinicor SX+


Fig. 4. (d) SMF-28e+
Figure 5 depicts the results of an experiment conducted in 2011 at BNL, in which fibers were tested at $-25^{\circ} \mathrm{C}$ to a dose of $10 \mathrm{kGy}(\mathrm{Si})$ at a dose rate of $\sim 60 \mathrm{~Gy}(\mathrm{Si}) / \mathrm{hr}$. In this experiment, two new fibers, the SMF-28XB (SM) and ClearCurve OM3 (MM), were tested, as they could potentially render some of the previously-tested fibers obsolete. These same two fibers performed better than their older counterparts, the SMF-28 (SM) and Infinicor SX+ (MM). The ClearCurve experienced a maximum RIA of $0.03 \mathrm{~dB} / \mathrm{m}$, while the SMF-28XB experienced a peak RIA of $0.057 \mathrm{~dB} / \mathrm{m}$ [12]. However, all of the fibers tested were qualified for low-dose operations at the LHC. As a side note, one of the ClearCurve fibers, labelled OSA in the Figure, was removed during the course of the experiment for other purposes.


Fig. 5. RIA of fibers for the 2011 BNL experiment

## 4. Conclusions

Since 2008, the Versatile Link Project has tested multiple optical fibers for use in fiber optic data links, as part of the proposed LHC upgrades. Two MM fibers (the Infinicor SX+ and Draka-RHP-1) and one SM fiber (SMF-28) have been qualified for warm operations at the LHC. Two SM fibers (Fibres X and Y) were qualified for low-temperature operations at the LHC in a high-dose test. During this experiment, the MM fibers experienced very high RIA. The Infinicor SX+, despite experiencing high RIA at a high dose rate, is still a viable MM candidate; it exhibits low RIA at a low dose rate, and the dose rate used in the high dose experiment was far higher than the $\sim 9 \mathrm{~Gy}(\mathrm{SI}) / \mathrm{hr}$ that the fiber would experience in operation at the LHC. The newer ClearCurve OM3 and SMF-28XB perform even better at a low dose rate than their older counterparts, but still must be tested at high doses. Another fiber radiation test was conducted during the summer of 2011, subjecting fibers to a relatively high radiation dose of 220 $\mathrm{kGy}(\mathrm{Si})$, but at a lower dose rate. The results are currently being analyzed. All of these experiments contribute to the knowledge pool of radiation-tolerant optical fibers, opening the door for applications in particle physics, space exploration, and many other scientific endeavors.

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# Electron and photon reconstruction and identification in ATLAS: expected performance at high energy and results at 900 GeV 

The ATLAS Collaboration


#### Abstract

This note presents the first study of electron and photon candidates in the 900 GeV collision data collected by ATLAS at the end of 2009, the collision events analysed corresponding to a total integrated luminosity of approximately $9 \mu b^{-1}$. Good agreement is demonstrated between observation and expectation for low- $p_{T}$ electron and photon reconstruction and identification. The expected performance of the reconstruction and identification algorithms used for this purpose and optimised for high- $p_{T}$ physics are described for reference in the first part of this note.


## 1 Introduction

At the end of 2009, ATLAS enjoyed a series of stable LHC runs at a centre-of-mass energy of 900 GeV , successfully recording and analysing the many collisions which took place. A significant number of low- $p_{T}$ electron and photon candidates were reconstructed in these events, the majority being ascribed to photons from $\pi^{0}$ decays, electrons from photon conversions, and hadrons faking electrons or photons. Whilst the transverse energies of the candidates observed in these data are well below those for which the reconstruction and identification algorithms have been optimised, the measurements already provide a quantitative test of both the algorithms themselves and the reliability of the performance predictions in the transverse energy range from the reconstruction threshold of 2.5 GeV to almost 10 GeV .

The electron and photon reconstruction and identification algorithms used in ATLAS are designed to achieve both a large background rejection and a high and uniform efficiency over the full acceptance of the detector and for transverse energies above 20 GeV . Isolated electrons need to be separated from hadrons in QCD jets, from background electrons (originating mostly from photon conversions in the tracker material), and from non-isolated electrons from heavy flavour decays. At transverse energies above 20 GeV , neutral hadron decays, mainly the decay $\pi^{0} \rightarrow \gamma \gamma$, are responsible for the majority of background photons. Section 2 of this note gives an overview of the expected performance for electrons and photons, covering reconstruction, identification and calibration.

In Section 3, this note describes the observed electron and photon candidates at 900 GeV , and compares them to those obtained from high-statistics samples of non-diffractive minimum bias simulation. Specifically, this section compares the observed and predicted distributions of the electromagnetic calorimeter and tracker observables and of the match between them. In the case of the simulation, the predicted background is broken down into its different components, and these are compared in the case of electrons to a data-driven determination of each of the two major background components.

## 2 Expected reconstruction and identification performance

The ATLAS electromagnetic (EM) calorimeter has a fine segmentation in both the lateral ( $\eta \times \phi$ space) and longitudinal directions of the showers [1]. At high energy, most of the EM shower energy is collected in the second layer which has a lateral granularity of $0.025 \times 0.025$ in $\eta \times \phi$ space. The first layer consists of finer-grained strips in the $\eta$-direction (with a coarser granularity in $\phi$ ), which offer excellent $\gamma-\pi^{0}$ discrimination. These two layers are complemented by a presampler layer placed in front with coarse granularity to correct for energy lost in the material before the calorimeter, and by a back layer behind, which enables a correction to be made for the tail of very highly energetic EM showers.

The transition region between the barrel and end-cap EM calorimeters, $1.37<|\eta|<1.52$, is expected to have poorer performance than the fiducial regions discussed in this note because of the large amount of material in front of the first active calorimeter layers. The presampler layer covers only the range $|\eta|<1.8$. The end-cap EM calorimeters (EMEC) are divided into two wheels, the outer and inner wheels covering the ranges $1.375<|\eta|<2.5$ and $2.5<|\eta|<3.2$, respectively. The forward calorimeters (FCal) cover the range $3.1<|\eta|<4.9$ and also provide some EM shower identification thanks to their longitudinal segmentation into three layers.

The ATLAS inner detector provides precise track reconstruction over $|\eta|<2.5$ [2]. It consists of three layers of pixel detectors close to the beam-pipe, four layers of silicon microstrip detectors (SCT) providing eight hits per track at intermediate radii, and a transition radiation tracker (TRT) at the outer radii,
providing about 35 hits per track (in the range $|\eta|<2.0$ ). The TRT also provides substantial discriminating power between electrons and pions over a wide energy range (between 0.5 and 100 GeV ). The pixel vertexing layer (also called the B-layer) is located just outside the beam-pipe at a radius of 50 mm , and provides precision vertexing and significant rejection of photon conversions (through a requirement of a track with a hit in this layer).

All performance numbers quoted in this section are based on simulated samples at $\sqrt{s}=10 \mathrm{TeV}$ and are calculated in the absence of pile-up. Electron and photon reconstruction begins with the creation of a preliminary set of clusters in the EM calorimeter. The size of these seed clusters corresponds to $3 \times 5$ cells in $\eta \times \phi$ in the middle layer of the EM calorimeter. Electron and photon reconstruction is seeded from such clusters with $E_{T}>2.5 \mathrm{GeV}$, using a sliding window algorithm over the full acceptance of the EM calorimeter.

### 2.1 Electron reconstruction

Electrons are reconstructed from the sliding window clusters if there is a suitable match with a track of $p_{T}>0.5 \mathrm{GeV}$. The "best" track is the one lying with an extrapolation closest in $(\eta, \phi)$ to the cluster barycentre in the middle EM calorimeter layer. These reconstructed electron candidates are then subjected to an identification procedure designed to ensure that true electrons are selected with a high and uniform efficiency, whilst background electrons from photon conversions and fake electrons from QCD jets are strongly suppressed. Electron candidates with $|\eta|>2.5$ are termed "forward" electrons; they lie outside the range of the ATLAS tracking systems and are therefore reconstructed using an alternative algorithm. Focus is given in what follows to central electron reconstruction (see Sections 2.6 and 3.5 for details of forward electron reconstruction). For the barrel EM calorimeter, the optimal cluster size for electron candidates is $3 \times 7$ cells in $\eta \times \phi$, whereas it is $5 \times 5$ cells for the end-cap EM calorimeters.

### 2.2 Photon reconstruction

Photons are reconstructed from the sliding window clusters if there is no reconstructed track matched to the cluster (unconverted photon candidates) or if there is a reconstructed conversion vertex matched to the cluster (converted photon candidates). Converted photon candidates are efficiently reconstructed only if the conversion radius is below 800 mm and high efficiency in this range can only be achieved if one considers, in addition to double-track conversions, the so-called single-track conversions, i.e. those for which only one track is reconstructed and does not have any hit in the B-layer (see ref. [3] for details). A large fraction of single-track conversion candidates corresponds to a track reconstructed only in the TRT detector. Such tracks have no associated silicon detector information and have therefore poorer momentum resolution and $\eta$ information.

For the barrel EM calorimeter, the optimal cluster size for unconverted photon candidates is $3 \times 5$ cells in $\eta \times \phi$ whereas it is $3 \times 7$ cells for converted photon candidates. For the end-cap EM calorimeters, the optimal cluster size is $5 \times 5$ cells for all photon candidates.

### 2.3 Electron-photon ambiguities

In order to maximise the electron and photon reconstruction efficiencies simultaneously, a significant fraction of the converted photon candidates are considered also as electrons. The fraction of these ambiguous candidates is large and varies with $\eta$ due to the material distribution in the tracker. Two examples are given here:

- approximately $0.9 \%$ of electrons with $E_{T}>20 \mathrm{GeV}$ and $|\eta|<2.5$ from $Z \rightarrow e e$ decay are not reconstructed at all and a larger fraction of $\sim 2.1 \%$ are reconstructed as photons. Among those reconstructed successfully as electron candidates, a significant fraction of $\sim 10.1 \%$ are ambiguous, and almost all of these are also reconstructed as converted photons;
- less than $0.1 \%$ of photons with $E_{T}>20 \mathrm{GeV}$ and $|\eta|<2.5$ from $H \rightarrow \gamma \gamma$ decay ( $m_{H}=120 \mathrm{GeV}$ ) are not reconstructed at all and a larger fraction of $\sim 2.1 \%$ are reconstructed as electrons. Among those reconstructed successfully as photon candidates, a large fraction of $\sim 42.1 \%$ are ambiguous, and about $72.5 \%$ of these are reconstructed as converted photons. Approximately $93.5 \%$ of the converted photons are also reconstructed as electrons.

Since these ambiguous candidates often correspond to early showers in the tracker material, the efficiency of the identification cuts described below may be significantly reduced relative to the rest of the electrons and photons.

### 2.4 Calibration

In addition to identifying efficiently EM showers, the ATLAS EM calorimeter measures their energies with high accuracy and with a linearity better than $0.5 \%$ over a large energy range, from 10 GeV to a few TeV . The procedure to measure the energy of an incident electron or photon is described in detail in [4]. Each step of the energy reconstruction has been validated by a series of beam tests over several years, using not only the calorimeter alone [5], but also a combination of representative components from the tracker in front of the barrel calorimeter [6]. This has led to considerable refinements of the calorimeter simulation, which has been used in recent years to model the behaviour of the full detector in situ and to provide precise calibration corrections over the full pseudorapidity and energy range required. One of the key ingredients for the description of the detector performance is the amount and position of the upstream material (tracker material, cryostats, solenoid coil).

The cluster energy is determined precisely by computing and summing four different contributions: the energy deposited in the material in front of the EM calorimeter (including the energy between the cold calorimeter wall and the first accordion compartment), that deposited in the calorimeter inside the cluster, that deposited outside the cluster (lateral leakage) and the energy deposited beyond the EM calorimeter (longitudinal leakage). The four terms are parametrised as a function of the cluster measured energies in the presampler (where it is present) and in the three accordion longitudinal layers. The parameters are computed at each pseudorapidity value corresponding to the centre of a cell in the middle layer. Symmetry between positive and negative pseudorapidity values and in azimuth is assumed.

Figure 1 shows the linearity of the response, defined as the ratio between the reconstructed and the true particle energy, for different particle types as a function of pseudorapidity and at different energies. The deviation from linearity is less than $\pm 0.5 \%$ for electrons and unconverted photons at almost all values of $|\eta|$. For converted photons, the deviation from linearity lies within $\pm 1 \%$ over most of the simulated samples, reaching $+1.5 \%$ at low energies in the interval $|\eta|=1.7-2.2$, where the material impact is largest (the last bin in pseudorapidity is missing for converted photons due to lack of statistics).

The fractional energy resolution $\sigma / E$ as a function of $|\eta|$ is shown in Fig. 2 for different energies and for electrons, converted and unconverted photons separately. The resolution deteriorates as a function of the number of radiation lengths in front of the EM calorimeter. This effect is particularly visible for the lower-energy electrons and converted photons and is due to the combined effect of the bremsstrahlung radiation and the magnetic field. At large values of $|\eta|$, the resolution is similar to the one obtained in the


Figure 1: Expected linearity of response of the EM calorimeter for electrons (a), converted photons (b) and unconverted photons (c) as a function of pseudorapidity.


Figure 2: Expected fractional energy resolution of the EM calorimeter for electrons (a), converted photons (b) and unconverted photons (c) of different energies as a function of pseudorapidity.


Figure 3: Expected fraction of electrons (a), converted photons (b) and unconverted photons (c) with an energy measured in the EM calorimeter more than $1.5 \sigma$ below the fitted value of the Gaussian mean as a function of pseudorapidity and energy.
central region. The resolution at high energies $(\geq 200 \mathrm{GeV})$ is $\sim 1 \%$ over the whole $|\eta|$ range, dominated by an estimated global constant term of $0.7 \%$.

The energy resolution shown in Fig. 2 corresponds to the fitted gaussian core of the distribution; the non-gaussian nature of the energy losses due to bremsstrahlung and the magnetic field make it important to illustrate the expected performance additionally in terms of the fraction of events with measured energy significantly below the true energy. The fraction of events with a reconstructed energy smaller than the true energy minus $1.5 \sigma$ is illustrated as a function of pseudorapidity for different particle types and different energies in Fig. 3. The fraction of events in the tails approaches the value expected for a gaussian distribution for the low $|\eta|$ and high-energy points, but it is significantly higher at lower energies and higher pseudorapidity values.

### 2.5 Electron and photon identification

The baseline electron and photon identification algorithms in ATLAS rely on rectangular cuts using variables which deliver good separation between isolated electrons/photons and fake signatures from QCD jets. These variables include information from the calorimeter and, in the case of electrons, tracker and combined calorimeter/tracker information. Three reference sets of cuts have been defined for electrons: loose, medium and tight, and two sets for photons: loose and tight, as listed in Table 1. The cut values are optimised in bins of $E_{T}$ and $\eta$ for electrons and only in bins of $\eta$ for photons, but separately for unconverted photons and converted photons.

For trigger purposes, electrons and photons share a common set of loose cuts and cut thresholds. This basic selection includes shower-shape variables based on information from the middle calorimeter layer, together with hadronic leakage, the fraction of the cluster energy deposited in the hadronic calorimeter layers (see Table 1) beyond the EM calorimeter. Although these loose cuts are shared, the electron candidates will consist of clusters associated to a loosely matching track whereas the photon candidate clusters will in general lack such a track. Photon identification rejects $\pi^{0}$ decays using the fine granularity of the first layer of the EM calorimeter. Consequently, photon candidates are required to lie within $|\eta|<2.37$. Electron candidates are required to lie within the region covered by the tracker and the precision region of the EM calorimeter, $|\eta|<2.47$.

Loose electron candidates can be selected further using the medium selection, which consists of requirements on their energy deposits in the strip layer of the EM calorimeter and on the track quality and track-cluster match. The tight electron requirements are explicitly optimised to exploit the full potential of the ATLAS electron identification with the purpose of specifically rejecting charged hadrons, by using the ratio between measured cluster energy and track momentum, $\mathrm{E} / \mathrm{p}$, and the fraction of high-threshold hits in the TRT, and background electrons from photon conversions, by requiring the presence of a hit on the track in the pixel vertexing layer and rejecting candidates with a matching conversion vertex. They also comprise tighter track-matching cuts and impact parameter cuts. For robustness, cut choices (including thresholds) are based on the expected level of understanding of the detector performance at start-up.

The tight photon requirements are also optimised to provide good rejection of the most dangerous background consisting of isolated leading $\pi^{0} \mathrm{~s}$. They comprise tighter cuts on the variables used for the loose cut selection and additional cuts on the middle layer and especially the strip layer with its fine granularity which provides good $\gamma-\pi^{0}$ separation. A more detailed description of the identification cuts can be found in refs. [7] and [8] for electrons and photons, respectively.

Table 1: Definition of variables used for all electron and photon identification cuts.

| Type | Description | Name |
| :---: | :---: | :---: |
| Loose electron and photon cuts |  |  |
| Acceptance of the detector | $\|\eta\|<2.47$ for electrons, $\|\eta\|<2.37$ for photons (1.37<\| $\eta \mid<1.52$ excluded) | - |
| Hadronic leakage | Ratio of $E_{T}$ in the 1st sampling of the hadronic calorimeter to $E_{T}$ of the EM cluster (used over the range $\|\eta\|<0.8$ and $\|\eta\|>1.37$ ) Ratio of $E_{T}$ in the hadronic calorimeter to $E_{T}$ of the EM cluster (used over the range $\|\eta\|>0.8$ and $\|\eta\|<1.37$ ) | $\begin{aligned} & R_{\text {had } 1} \\ & R_{\text {had }} \end{aligned}$ |
| Middle layer of the EM calorimeter | Ratio in $\eta$ of cell energies in $3 \times 7$ versus $7 \times 7$ cells. Lateral width of the shower | $\begin{aligned} & R_{\eta} \\ & w_{2} \end{aligned}$ |
| Medium electron cuts (in addition to the loose cuts) |  |  |
| Strip layer of the EM calorimeter | Total lateral shower width (20 strips) <br> Ratio of the energy difference between the largest and second largest energy deposits over the sum of these energies | $w_{\text {stot }}$ <br> $E_{\text {ratio }}$ |
| Track quality | Number of hits in the pixel detector (at least one) Number of hits in the pixels and SCT (at least seven) Transverse impact parameter $(<5 \mathrm{~mm})$ | $\begin{aligned} & - \\ & - \\ & d_{0} \end{aligned}$ |
| Track matching | $\Delta \eta$ between the cluster and the track in the strip layer of the EM calorimeter | $\Delta \eta_{1}$ |
| Tight electron cuts (in addition to the medium electron cuts) |  |  |
| B-layer | Number of hits in the B-layer (at least one) |  |
| Track matching | $\Delta \phi$ between the cluster and the track in the middle layer of the EM calorimeter Ratio of the cluster energy to the track momentum | $\begin{aligned} & \Delta \phi_{2} \\ & \mathrm{E} / \mathrm{p} \\ & \hline \end{aligned}$ |
| TRT | Total number of hits in the TRT (used over the acceptance of the TRT, $\|\eta\|<2.0$ ) <br> Ratio of the number of high-threshold hits to the total number of TRT hits (used over the acceptance of the TRT, $\|\eta\|<2.0$ ) | - |

Tight photon cuts (in addition to the loose cuts, applied with stricter thresholds)

| Middle layer of the | Ratio in $\phi$ of cell energies |  |
| :--- | :--- | :--- |
| in $3 \times 3$ and $3 \times 7$ cells |  | $R_{\phi}$ |
| EM calorimeter | Shower width for three strips around maximum strip |  |
| Strip layer of the | Total lateral shower width | $w_{s 3}$ |
| EM calorimeter | Fraction of energy outside core of three central strips but within seven strips | $w_{\text {stot }}$ |
|  | Difference between the energy of the strip with the second largest |  |
|  | energy deposit and the energy of the strip with the smallest energy deposit between | $\Delta E$ |
|  | the two leading strips |  |
|  | Ratio of the energy difference associated with the largest and second largest |  |
|  | $E_{\text {ratio }}$ |  |

### 2.5.1 Expected performance

The electron or photon identification efficiency is defined as:

$$
\begin{equation*}
\varepsilon_{e, \gamma}^{\text {truth }}=\frac{N_{e, \gamma}^{\text {reco }}}{N_{e, \gamma}^{\text {truth }},} \tag{1}
\end{equation*}
$$

where $N_{e, \gamma}^{\text {truth }}$ is the total number of true electrons or photons within the acceptance of simple kinematic cuts on transverse energy and pseudorapidity, and $N_{e, \gamma}^{r e c o}$ is the number of reconstructed signal electrons or photons passing identification cuts. The quoted jet rejections are normalised with respect to the number of truth particle jets. The jet rejection is defined as:

$$
\begin{equation*}
R_{\mathrm{jet}}=\frac{N_{\text {truth jets }}}{N_{\text {fakes }}}, \tag{2}
\end{equation*}
$$

where $N_{\text {truth }}$ jets is the number of true jets in the initial sample and $N_{\text {fakes }}$ is the number of candidates passing a specific selection. Truth jets are defined by summing particle four-momenta within a cone size $\Delta R=0.4$ and the number of truth jets per event is derived from an unfiltered sample of important hard processes, mainly di-jet events (referred to loosely in what follows as di-jets). The total number of truth jets is then obtained through:

$$
\begin{equation*}
N_{\text {truth jets }}=N_{\text {total }} \times F_{\text {jets }}, \tag{3}
\end{equation*}
$$

where $N_{\text {total }}$ is the number of events used in the analysis and $F_{\text {jets }}$ the number of truth jets per generated event.

The electron efficiencies and jet rejections, for $E_{T}>20 \mathrm{GeV}$ and averaged over $|\eta|$, are given in Table 2 for the loose, medium and tight selections. Figure 4 shows in more detail how the overall efficiency of each set of cuts varies with $E_{T}$ and $|\eta|$. Not surprisingly, because of the large amount of material in the tracker and in front of the EM calorimeter, the efficiency is lower at intermediate pseudorapidity values and decreases rapidly for transverse energies below $\sim 15 \mathrm{GeV}$. Nevertheless, medium cuts are expected to have an efficiency approaching $90 \%$. Table 2 also shows that the specific cuts optimised for the tight selection successfully remove the large backgrounds from hadrons and converted photons, which are largely dominant after the medium selection. The resulting sample should be dominated by prompt electrons, most of them non-isolated electrons from $b, c$ decays and a significant fraction of them isolated electrons from decays of $W / Z$ bosons.

The corresponding results for the loose and tight photon selections are shown in Table 3 and in Fig. 5. The overall efficiency of the tight selection decreases rapidly for transverse energies below $\sim 30 \mathrm{GeV}$. The jet rejections shown in Table 3 are averaged over the jet flavours expected in di-jet events with $E_{T}>20 \mathrm{GeV}$. It is important to note that the rejection expected against gluon jets is higher by a factor of $\sim 5$ than that expected against light-quark jets because of the broader and softer fragmentation properties of gluon jets. The specific cuts based on the strip-layer information provide a rejection of a factor of three against isolated $\pi^{0}$ decays.

### 2.6 Forward electrons

Electron identification in the forward region $(|\eta|>2.5)$ will be important in many physics analyses, including electroweak measurements and searches for new phenomena. In the range $2.5<|\eta|<4.9$ the calorimeters are the only source of information (the ATLAS tracking system being limited to the range $|\eta|<2.5$ ). Therefore such electrons can only be identified clearly above the background in specific topologies, such as $Z \rightarrow e e$ or $H \rightarrow e e e e$ decays. Electron candidates in the forward calorimeters are

Table 2: Expected jet rejections with overall isolated and non-isolated electron efficiencies for the three sets of identification cuts and an $E_{\mathrm{T}}$-threshold of 20 GeV . The total jet rejection includes hadron fakes and background electrons from photon conversions and Dalitz decays. The last four columns give the fraction of surviving electron candidates in the di-jet sample after each selection level. Isolated electrons correspond to electrons from $W, Z$ decays, non-isolated electrons to heavy flavour semi-leptonic decays and background electrons originate from photon conversions and Dalitz decays. Hadrons denote the remaining QCD jet background, which is dominated by charged hadrons faking an electron signature. The quoted errors are statistical.

|  | Efficiency (\%) |  | Jet rejection (total) | Surviving candidates in jets (percentage of total) |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $Z \rightarrow e e$ | $b, c \rightarrow e$ |  | Isolated <br> electrons | Non-isolated <br> electrons | Background <br> electrons | Hadrons |
| Reconstructed | $97.56 \pm 0.03$ | - | $91.5 \pm 0.1$ | 0.1 | 0.8 | 23.3 | 75.8 |
| Loose | $94.30 \pm 0.03$ | $36.8 \pm 0.5$ | $1066 \pm 4$ | 1.0 | 2.0 | 56.7 | 40.3 |
| Medium | $89.97 \pm 0.03$ | $31.5 \pm 0.5$ | $6821 \pm 69$ | 5.9 | 9.8 | 50.7 | 33.6 |
| Tight | $71.52 \pm 0.03$ | $25.2 \pm 0.5$ | $(1.38 \pm 0.06) \times 10^{5}$ | 29.6 | 44.8 | 11.5 | 14.1 |



Figure 4: Expected electron efficiency versus $|\eta|(a)$ and $E_{T}$ (b) shown for loose, medium and tight selection criteria.
reconstructed based on EM topological clusters with $E_{T}>5 \mathrm{GeV}$. The direction of the electron is defined by the barycentre of the cells belonging to the calorimeter cluster. The electron candidates in this region correspond to clusters reconstructed in the end-cap EM calorimeter (EMEC) and the hadronic end-cap calorimeter behind it in the range $2.5<|\eta|<3.2$ and to clusters reconstructed much further away from the interaction point in the forward calorimeters (FCal) in the range $3.1<|\eta|<4.9$. In both ranges, the total cluster energy reconstructed in the calorimeters is taken to be that of the electron candidate.

In order to distinguish electrons from hadrons, the differences between their EM showers must be exploited. These differences are apparent in the energy deposition and the shower shapes produced by the two types of particles. The good transverse and longitudinal calorimeter segmentation provides additional particle identification capability. Most of the variables used in the identification algorithm are the individual cluster moments themselves or a combination of these moments.

Table 3: Expected overall photon efficiencies and jet background rejections for the two sets of identification cuts and an $E_{T}$-threshold of 20 GeV .

|  |  | Efficiency (\%) | Jet rejection |
| ---: | ---: | :--- | :---: |
|  | All | $95.45 \pm 0.01$ | $908 \pm 4$ |
| Loose | Unconverted | $97.80 \pm 0.01$ |  |
|  | Converted | $91.73 \pm 0.01$ |  |
|  | All | $82.88 \pm 0.02$ | $4770 \pm 40$ |
| Tight | Unconverted | $85.04 \pm 0.03$ |  |
|  | Converted | $79.44 \pm 0.04$ |  |



Figure 5: Expected photon efficiency vs $|\eta|$ (left) and $E_{T}$ (right) for loose and tight selection criteria and for unconverted (top) and converted (bottom) photons.

## 3 Results from collisions at $900 \mathbf{~ G e V}$

### 3.1 Event samples

The analysis is based on a data sample collected at $\sqrt{s}=900 \mathrm{GeV}$. The events are triggered during LHC stable beams using the Minimum-Bias-Trigger-Scintillators (MBTS), which cover the pseudorapidity range, $2.09<|\eta|<3.84$, and are located in front of the end-cap EM calorimeters. Collision candidates are selected using additional timing requirements to provide further rejection against beam backgrounds: either coincident signals from the EM calorimeter end-caps or from the MBTS. Events are selected for which the tracker, electromagnetic calorimeter and hadronic calorimeters recorded data with high quality and the solenoidal field was at its nominal value. The obtained data sample consists of 384,186 collision candidates and corresponds to an integrated luminosity of approximately $9 \mu b^{-1}$. The Monte Carlo event sample used throughout this note is composed of $10^{7}$ non-diffractive minimum bias events generated with Pythia, using the ATLAS mc09 tune [9], and passed through the full ATLAS simulation and reconstruction software. The contribution from single and double diffractive events is negligible in this regime.

This study considers all reconstructed electron and photon candidates with cluster $E_{T}>2.5 \mathrm{GeV}$. Initially, electron candidates with a cluster $|\eta|<2.47$ and photons with cluster $|\eta|<2.37$ are selected and investigated (the cluster $\eta$ is defined here as the barycentre of the cluster cells in the middle layer of the EM calorimeter). A separate study of forward electrons then follows in Section 3.5, these electron candidates satisfying $|\eta|>2.5$. Electron and photon candidates in the EM calorimeter transition region $(1.37<|\eta|<1.52)$ are not considered. In what follows, the barrel region is defined as the range $|\eta|<1.37$ and the end-cap region as the range $1.52<|\eta|<2.37$ for photons and $1.52<|\eta|<2.47$ for electrons. For the comparisons presented here, the Monte Carlo distributions are always normalised to the sample of data events.

### 3.2 Electron candidates

Table 4 presents the numbers of reconstructed electron candidates, over the full acceptance and in each region defined above, as a function of the selection cuts applied. These selection cuts are not optimised for such low-energy electron candidates (see Section 2.5). Figure 6 displays for all selected electron candidates the transverse energy and pseudorapidity spectra. Both Table 4 and Fig. 6 show agreement between data and simulation, given the large uncertainties expected in the kinematic regime considered here. The Monte Carlo sample is sub-divided into its two dominant components: hadrons and electrons from conversions, as shown in Fig. 6. The latter component corresponds to $\sim 33 \%$ of all the electron candidates and is largely dominated by electrons from photon conversions, but also includes a small component ( $\sim 3 \%$ ) of background electrons from other sources, such as Dalitz decays, and an even smaller one (below $1 \%$ ) of prompt electrons from $b, c \rightarrow e$ decays. As can be seen in Table 4, the fractions of hadrons and conversions expected, as a function of the cuts applied and the $\eta$-range considered, vary according to the amount of material in the tracker and to the specific kinematic features of these backgrounds at these low transverse energies. The low statistics available here do not allow quantitative comparisons of variables between data and simulation after tight selection cuts, for which the expectation is that a significant fraction of the electron candidates in Table 4 are prompt electrons from $b, c$ decay. Approximately $15 \%$ of the Monte Carlo electron candidates passing the tight cuts are expected to be prompt electrons, which means that three out of the twenty electron candidates passing tight cuts in the data would be expected to originate from heavy flavour decay. In the following, distributions will be compared between data and simulation for all selected candidates unless specified otherwise.

Table 4: Breakdown of electron candidates according to identification cuts applied and to $\eta$-range: the whole $\eta$-range is considered (left), as well as the $\eta$-ranges of the barrel (middle) and end-cap (right) EM calorimeters. The first row gives the total numbers of electron candidates reconstructed in data in the three different $\eta$-ranges. For each of these $\eta$-ranges, the percentages of identified loose, medium and tight candidates in data are compared to those predicted by Monte Carlo (MC). The numbers in brackets give the percentage of Monte Carlo electron candidates which are electrons from photon conversions or prompt electrons (the remainder are charged hadrons).

| Electron <br> candidates | All <br> 879 |  | Barrel <br> 558 |  | Endcap <br> 321 |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Data (\%) | MC (\%) | Data (\%) | MC (\%) | Data (\%) | MC (\%) |
| Loose | $46.5 \pm 1.7$ | $50.9 \pm 0.2(40.0 \pm 0.3)$ | $47.3 \pm 2.1$ | $51.8 \pm 0.3(33.1 \pm 0.4)$ | $45.2 \pm 2.8$ | $49.5 \pm 0.4(51.2 \pm 0.5)$ |
| Medium | $10.6 \pm 1.0$ | $13.1 \pm 0.2(26.4 \pm 0.6)$ | $11.1 \pm 1.3$ | $12.9 \pm 0.2(19.5 \pm 0.7)$ | $9.6 \pm 1.6$ | $13.3 \pm 0.3(36.9 \pm 1.0)$ |
| Tight | $2.3 \pm 0.5$ | $2.4 \pm 0.1(37.9 \pm 1.5)$ | $1.6 \pm 0.5$ | $1.8 \pm 0.1(49.2 \pm 2.2)$ | $3.4 \pm 1.0$ | $3.3 \pm 0.1(28.7 \pm 1.8)$ |



Figure 6: Cluster $E_{T}$ (a) and $|\eta|$ (b) for all selected electron candidates.

### 3.3 Photon candidates

Table 5 presents the numbers of reconstructed photon candidates, over the full acceptance and in each region defined above, as a function of the selection cuts applied. A total fraction of only $14 \%$ of the photon candidates are reconstructed as converted photons and almost all of them, $\sim 98 \%$, are ambiguous and also reconstructed as electron candidates, which is not surprising at these low energies since the two electrons from conversions rarely end up with their energy collected in a single EM cluster. Transverse energy and pseudorapidity spectra for all selected photon candidates are displayed in Fig. 7 and found to be in agreement between data and Monte Carlo. The Monte Carlo sample is sub-divided in this case into four components of decreasing importance: approximately $71 \%$ of the candidates correspond to photons from $\pi^{0}$ decay, whereas $\sim 14 \%$ are from $\eta, \eta^{\prime}$ or $\omega$ decay into two photons, and $\sim 14 \%$ are from other hadrons with complex decay processes and particles interacting in the tracker material. Only a very small fraction of $\sim 0.7 \%$ of all photon candidates are expected to be "prompt" at these energies, i.e. from initial or final state radiation of quarks. Other sources of prompt photons, e.g. from $p p \rightarrow \gamma+\mathrm{jet}$, are not included in the Monte Carlo. In the following, as in the case of the electron candidates discussed above, the distributions will be compared between data and simulation for all selected candidates unless specified otherwise.

Table 5: Breakdown of photon candidates according to identification cuts applied and to $\eta$-range considered: the whole $\eta$-range is considered (left), as well as the $\eta$-ranges of the barrel (middle) and end-cap (right) EM calorimeters. The first row gives the total numbers of photon candidates reconstructed in data in the three different $\eta$ ranges. For each of these $\eta$-ranges, the percentages of identified loose and tight candidates in data are compared to those predicted by Monte Carlo (MC).

| Photon <br> candidates | 1694 |  | Barrel <br> 1247 |  | Endcap <br> 447 |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Data (\%) | MC (\%) | Data (\%) | MC (\%) | Data (\%) | MC (\%) |
| Loose | $25.4 \pm 1.0$ | $30.5 \pm 0.1$ | $24.3 \pm 1.2$ | $29.0 \pm 0.1$ | $28.4 \pm 2.1$ | $34.3 \pm 0.3$ |
| Tight | $4.1 \pm 0.5$ | $6.6 \pm 0.1$ | $3.6 \pm 0.5$ | $5.3 \pm 0.1$ | $5.8 \pm 1.1$ | $9.9 \pm 0.2$ |



Figure 7: Cluster $E_{T}(a)$ and $|\eta|$ (b) for all selected photon candidates.

### 3.4 Electron and photon identification

### 3.4.1 Calorimeter variables

In this section, various calorimeter variables are illustrated for the photon candidates, the equivalent distributions for electron candidates display very similar features. Figure 8 illustrates the longitudinal development of the shower in the successive layers of the EM calorimeter, based on the measured layer energies before cluster corrections are applied. For the observed photon candidates before identification cuts, which almost all have transverse energies below 10 GeV and correspond predominantly to photons from $\pi^{0}$ decays, approximately half of the total energy ( $55 \%$ ) is deposited on average in the middle layer, a third in the strip layer, and $9 \%$ in the presampler (a negligible amount is deposited in the back layer). In the presampler part, a noticeable disagreement between data and simulation can be seen for values higher than 0.6. In the simulation, this part of the distribution is populated mostly by hadrons. This feature also explains the observed small but systematic disagreement in the first bins for the fractions in the other layers, since the various fractions are correlated.

The fraction of the cluster energy deposited in the first layer of the hadronic calorimeter (or hadronic leakage) is shown in Fig. 9(a), demonstrating agreement between data and simulation. This is not surprising for the low cluster energies discussed here, since most of the energy is deposited in the first layers of the EM calorimeter (see Fig. 8) and the hadronic leakage is clearly dominated by noise. The lateral development of the shower, as detailed by the variables $w_{2}, R_{\eta}$ and $R_{\phi}$ described in Section 2.5 and


Figure 8: Fraction of energy deposited by photon candidates in each layer of the electromagnetic calorimeter for data and simulation. These fractions are labelled as $f_{0}$ for the presampler layer (a), $f_{1}$ for the strip layer ( $b$ ), $f_{2}$ for the middle layer ( $c$ ) and $f_{3}$ for the back layer (d).
in Table 1 [8], is illustrated for the photon candidates in Figs. 9(b)-(d). These variables all display small shifts between the shapes observed in data and those expected from simulation. The shower width $w_{2}$ is slightly larger in the data: preliminary studies show that including the cross-talk between neighbouring middle layer cells $(\sim 0.5 \%)$ [10] in the simulation would explain part of the observed difference.

The most illustrative shower-shape variables in the strip layer of the EM calorimeter are presented in Fig. 10 for all photon candidates. At the low energies measured in these data, the variables $\Delta E$ and $E_{\text {ratio }}$ (Figs. 10(a) and 10(b)) are mainly sensitive to the noise description. As discussed for the middle layer, the variables sensitive to the shower lateral width in the strip layer, $F_{\text {side }}$ and $w_{s 3}$, display distributions shifted slightly towards higher values in the data than in the simulation. The current simulation accounts for the measured cross-talk of $\sim 5 \%$ between neighbour strips and of $\sim 0.1 \%$ between middle and strip cells, as obtained from test-beam measurements [10]. Figure 11 shows comparisons between data and simulation for the lateral profile of the shower in the strips. Compared in Fig. 11(a) are the distributions of 3 GeV energy test-beam electrons at $\eta \sim 0.44$ and of the corresponding single electron MC simulation. In Figures 11(b) to 11(d) all photon candidates in the collision events are compared to the non-diffractive minimum bias MC events for three different $\eta$ regions. The lateral profiles of the


Figure 9: Distributions of calorimeter variables compared between data and simulation for all photon candidates. Shown are the hadronic leakage in the first layer of the hadronic calorimeter (a), the variables used for the loose selection cuts in the middle layer of the EM calorimeter, $w_{2}(b)$ and $R_{\eta}(c)$, and the variable used in tight selection, $R_{\phi}(d)$, as explained in Table 1.
showers for the test-beam (Fig. 11(a)) and for collision events with $|\eta|<0.8$ (Fig. 11(b)) are in good agreement between data and simulation. This agreement degrades significantly as $\eta$ varies, as can be seen in Figs. 11(c) and 11(d). This disagreement, a slightly wider distribution observed for data than for simulation, could account for a large fraction of the differences observed in Figs. 10(c) and 10(d) between the collision data and the simulation. Neither an inaccurate cross-talk description (the effect observed is too large) nor an incorrect description of the material in front of the EM calorimeter (different set-ups in the test-beam and in ATLAS itself) are likely to explain entirely this effect. In the end-cap, however, the amount of upstream material is likely to be one of the most significant causes of the observed discrepancies. More data will be required to understand whether a combination of such effects, an incorrect modelling of the simulation of the EM calorimeter, or an insufficiently accurate simulation of the physics processes in the shower simulation are responsible for these effects.


Figure 10: Distributions of shower-shape variables in the strip layer of the EM calorimeter compared between data and simulation for all photon candidates. Shown are several of the variables used for the tight photon cuts, $\Delta E(a), E_{\text {ratio }}(b), F_{\text {side }}(c)$ and $w_{s 3}(d)$, as explained in Table 1.

### 3.4.2 Tracking and track-cluster matching variables

Electron and converted photon reconstruction and identification rely heavily on tracking performance. Figure 12 illustrates two of the track-calorimeter matching variables used in identification for all electron candidates reconstructed in data and simulation. Figure 12(a) shows the difference in azimuth, $\Delta \phi_{2}$, between the track extrapolated to the middle layer of the EM calorimeter and the barycentre of the cell energies in this layer. In order to optimise the efficiency of the matching cut in the frequent case of large energy losses due to bremsstrahlung in the tracker material, this matching variable is sign-corrected to account for the opposite curvatures of electrons and positrons in the magnetic field and an asymmetric cut is applied in the selection to keep most of the candidates with large negative $\Delta \phi_{2}$. In contrast and as expected, Figure 12(b), which shows the difference in $\eta, \Delta \eta_{1}$, between the track extrapolated to the strip layer of the EM calorimeter and the barycentre of the cell energies in this layer, does not display any significant asymmetric tails due to bremsstrahlung. The two main components of the background, namely hadrons and electrons from conversions are also shown in Fig. 12: as expected, the asymmetric tails at large negative values of $\Delta \phi_{2}$ are more pronounced for the electrons than for the hadrons, whereas such tails do not appear in the $\Delta \eta_{1}$ distribution.


Figure 11: Lateral shower profile in the strip layer for 3 GeV electrons at $\eta \sim 0.44$ in test beam and simulation (a) and for all photon candidates in collision data and simulation for three $\eta$-ranges (b), (c), (d). The histograms are normalised to the bin with the highest value.

Figure 13 shows four of the tracking variables compared between data and simulation for all electron candidates. The agreement between data and simulation is good for all four distributions, despite the complications expected at these low energies due to material effects and track reconstruction inefficiencies. Figures 13(a) and 13(b) show the numbers of hits on the reconstructed tracks in the pixel and SCT detectors, respectively. As expected, a large fraction of the electrons from conversions in the simulation correspond to tracks with no hits in these detectors. A significant fraction of the hadrons also have no hits in these detectors, indicating that the track-matching algorithm is picking up tracks from secondaries in the TRT detector. Figure 13(c) displays the fraction of high-threshold TRT hits belonging to the track for electron candidates with $|\eta|<2.0$ and with a total number of TRT hits larger than ten: even at these low energies for which the transition radiation yield of electrons is not optimal, a very clear difference can be seen between the distributions expected for hadrons (lying mostly at low values of this fraction) and for electrons from conversions (a large fraction of which lie at high values of this fraction). Finally, Fig. 13(d) shows the distribution of the transverse impact parameter, $d_{0}$, of the electron track with respect to the reconstructed primary vertex position in the transverse plane: whereas the hadrons in the simulation display a distribution peaked around zero with a resolution of $\sim 100 \mu \mathrm{~m}$, the electrons from conversions have large impact parameters, which is to be expected from conversions occurring at


Figure 12: Distributions of track-calorimeter matching variables in $\phi$ (a) and $\eta$ (b) for all electron candidates compared between data and simulation.
large radii.

Figure 14(a) shows the distribution of the ratio E/p of cluster energy in the calorimeter to track momentum for all electron candidates and for data and simulation. The simulation shows that the expected peak from the electron component lies slightly above unity, with a tail expected toward high values of $\mathrm{E} / \mathrm{p}$ from bremsstrahlung losses in the tracker material. However, the observed peak shift and the extent of the high tail are not entirely due to bremsstrahlung losses. An additional contribution arises from an overestimate of the cluster energy, in the cases where it includes energy from nearby particles. The large fraction of electrons with small values of $\mathrm{E} / \mathrm{p}$ is due mostly to tracks reconstructed without silicon hits, which are poorly measured in the TRT detector (see Section 2.2 ). The hadron component surprisingly also peaks at values just below unity: this is simply due to the fact that hadrons reconstructed as electron candidates deposit most of their energy in the EM calorimeter at these low energies. In a similar fashion, Fig. 14(b) illustrates the properties of the reconstructed converted photon candidates in terms of the same E/p ratio, where the converted photon momentum is estimated from the combination of the track momenta for double-track conversions and from the track momentum measurement available for single-track conversions. As for the electron candidates, the tails at low $\mathrm{E} / \mathrm{p}$ are mostly due to tracks reconstructed only in the TRT detector. Approximately $20 \%$ of the converted photon candidates are reconstructed as single-track conversions in this kinematic regime.

### 3.4.3 Data-driven background estimation for electrons

As already discussed in Section 3.2, at the low energies considered here, the electron candidate data sample is expected to consist predominantly of two components: charged hadrons faking electrons, denoted here as $h \rightarrow e$, and electrons from photon conversions, denoted here as $\gamma \rightarrow e$. These two components can be separated in the data by using the known discriminatory power of the TRT between electrons and pions, based on the measured fraction of high-threshold TRT hits on the electron track (see Fig. 13(c)). To perform such a measurement, the electron candidates are required to lie within the TRT acceptance, i.e. $|\eta|<2.0$, and to have a reconstructed track with a total of at least ten TRT hits (no requirements are made on the number of silicon hits).


Figure 13: Distributions of tracking variables for all electron candidates compared between data and simulation. Shown are the number of pixel (a) and SCT (b) hits on the electron track, the fraction of high-threshold TRT hits for candidates with $|\eta|<2.0$ and with a total number of TRT hits larger than ten (c), and the transverse impact parameter, $d_{0}$, with respect to the reconstructed primary vertex (d).

This method has been applied to the electron data sample before identification cuts by separating the sample into a pion-enriched sub-sample with a fraction of high-threshold TRT hits below 0.06 and an electron-enriched sub-sample with a fraction of high-threshold TRT hits above 0.10 . The fraction of electrons falling into these sub-samples is predicted from simulation to be $6 \%$ for the pion-enriched sample and $80 \%$ for the electron-enriched sample. These fractions are predicted to be very different, $70 \%$ and $10 \%$ respectively, for pions. The response of the TRT to electrons and pions has been carefully modeled in the simulation based on test-beam measurements and varies significantly with energy and pseudorapidity in the kinematic regime consider here.

The respective efficiencies discussed above for pions and electrons to fall into these sub-samples are denoted by $\varepsilon_{T R<0.06}^{e, \pi}$ and $\varepsilon_{T R>0.10}^{e, \pi}$. If one defines the number of electron candidates of type $h \rightarrow e$ as $N^{\pi}$ and those of type $\gamma \rightarrow e$ as $N^{e}$, then one can predict the total number of electron candidates falling in the two categories above for the fraction of high-threshold TRT hits on the track:

$$
\begin{equation*}
N_{T R<0.06}=\varepsilon_{T R<0.06}^{e} N^{e}+\varepsilon_{T R<0.06}^{\pi} N^{\pi} \tag{4}
\end{equation*}
$$



Figure 14: Ratio, E/p, between cluster energy and track momentum for electron candidates (a) and for converted photon conversions (b).

$$
\begin{equation*}
N_{T R>0.10}=\varepsilon_{T R>0.10}^{e} N^{e}+\varepsilon_{T R>0.10}^{\pi} N^{\pi} \tag{5}
\end{equation*}
$$

The sample of 717 electron candidates considered here is thus predicted to contain 501 electron candidates of type $h \rightarrow e$ and 216 electron candidates of type $\gamma \rightarrow e$. Clearly, the extraction of these contributions can be refined as a function of the kinematic properties of the electron candidates (spectrum in $E_{T}$ and $\eta$ ). In addition, they can be compared to the composition found in the simulated events, in terms of the shapes predicted for electron identification variables which are not correlated to the identification through transition radiation. Such comparisons would provide a more precise validation of the agreement between data and simulation than that described in the previous sections since they would be obtained separately for each component of the sample.

Two examples of comparisons between the shapes of variables extracted for each of the two components, using the method described above (for each bin individually), and for the truth from simulation are shown in Figs. 15 and 16 respectively, for two of the most sensitive variables: the fraction of the cluster energy measured in the strip layer and the ratio $\mathrm{E} / \mathrm{p}$. The results are in good agreement, both in terms of the quite different shapes and the overall rates expected for each component. Clearly, more statistics will be required to probe the background components in more detail than outlined here.

The fraction of high-threshold TRT hits could be combined with the additional requirement of at least one B-layer hit associated to the reconstructed track to achieve a clean separation between the two components described here and the expected small fraction of prompt electrons from heavy flavour decays. In contrast to electrons from photon conversions, the latter are expected almost always to have a pixel hit measured on the track in the vertexing layer. With the statistics presented here, the estimated contribution from heavy flavours in the sample before identification cuts is consistent with zero within errors.

### 3.5 Forward electrons

Following the specific algorithm outlined in Section 2.6, a total of 369 forward electron candidates were reconstructed, with 234 candidates in the EMEC and 135 candidates in the FCal. These forward elec-


Figure 15: Distribution of the energy fraction in the strip layer of the EM calorimeter as extracted from data compared to the truth from simulation. The results are shown for both true (MC) and extracted (data) electrons from conversions (a) and hadron fakes (b).


Figure 16: Distribution of the E/p as extracted from data compared to the truth from simulation. The results are shown for both true (MC) and extracted (data) electrons from conversions (a) and hadron fakes (b).
tron candidates are predominantly photons and their transverse energy spectrum is shown in Fig. 17(a) for both data and simulation. Clusters induced by noise from problematic channels in the hadronic calorimeter are removed through a requirement that the energy fraction in the EM part of the cluster be greater than $0.5 \%$. Figure 17 (b) shows the second moment of the distance $R_{i}$ of each cell $i$ to the shower axis, which is sensitive to the lateral profile of the shower. The shower shape in the longitudinal direction is described by the second moment of the distance of each cell $i$ to the shower centre, as illustrated in Fig. 17(c). Finally, Fig. 17(d) displays the fraction of energy deposited in the EM layers of the calorimeters. The majority of candidates with a low EM-fraction are charged pions, whilst the majority of those with a high EM-fraction are photons from $\pi^{0} / \eta$ decays (as discussed in previous sections).


Figure 17: For forward electron candidates in data and simulation, distributions of transverse energy (a), of the lateral shower profile (b), the longitudinal shower profile (c) and the fraction of energy deposited in the EM layers of the calorimeters (d).

## 4 Conclusions

The data sample collected by ATLAS at $\sqrt{s}=900 \mathrm{GeV}$ at the end of 2009 has yielded samples of 879 electron candidates and 1694 photon candidates reconstructed with $E_{T}>2.5 \mathrm{GeV}$ before identification cuts. The performance of the reconstruction and identification algorithms on these data has been compared with expectations from simulation. Most of the features of the candidates are in remarkable agreement between data and simulation, including the background composition for electrons. This note also outlines the expected performance of the algorithms at the higher energies for which they have been optimised in terms of efficiency for the signal and rejection of the very large backgrounds expected from QCD jets.

Despite its limitations due to low statistics and the very low energies discussed here, this first experimental validation of the ATLAS electron and photon reconstruction and identification performance supports the expectation that the ATLAS inner detector and calorimeters will provide excellent data for electron and photon early physics at the LHC.

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# Photon Conversions at $\sqrt{s}=900 \mathrm{GeV}$ measured with the ATLAS Detector 

The ATLAS collaboration


#### Abstract

This note presents the first study of converted photons reconstructed with the ATLAS detector in the $\sqrt{s}=900 \mathrm{GeV}$ run in 2009. The analysis of the photon conversions demonstrates the excellent performance of the conversion reconstruction algorithm. The threedimensional distribution of the photon conversion vertices has been extracted and used to provide a first cross-check of the amount of material in the ATLAS tracker using collision data. A few Dalitz decays from neutral mesons have also been reconstructed and their rate is in agreement with expectations from simulation. Finally, the $\pi^{0}$ mass peak has been extracted from pairs of one converted and one unconverted photon.


## 1 Introduction

At the end of 2009, ATLAS enjoyed a series of stable LHC runs at a centre-of-mass energy of 900 GeV , successfully recording and analyzing the many collisions which took place. A significant number of low$p_{T}$ photon conversions were reconstructed and analyzed using dedicated algorithms. The reconstruction of electrons and of photon conversions is a particular challenge for the ATLAS inner detector, since electrons have lost on average between $20 \%$ and $50 \%$ of their energy (depending on their pseudorapidity $\eta$ ) when they leave the SemiConductor Tracker (SCT) and, in the same region, between $10 \%$ and $50 \%$ of photons convert into an electron-positron pair [1] [2].

This note describes in Section 3 the reconstruction of low- $p_{T}$ photon conversion candidates. This sample is used in Section 4 to compare its measured properties to those expected from simulation and to perform a first coarse estimate of the material in the inner tracking layers. Section 5 describes the few candidates found which are compatible with Dalitz decays of neutral mesons and Section 6 finally concludes with the extraction of a $\pi^{0}$ mass peak using one unconverted photon candidate and one photon conversion candidate.

## 2 The ATLAS Detector and Data Set

The ATLAS inner detector (ID) provides precise track reconstruction over $|\eta|<2.5$ [3]. It consists of three layers of pixel detectors close to the beam pipe, four layers of silicon microstrip detectors (SCT) providing eight hits per track at intermediate radii, and a transition radiation tracker (TRT) at the outer radii, providing about 30 hits per track (in the range $|\eta|<2.0$ ). The TRT also provides substantial discriminating power between electrons and pions over the wide energy range between 0.5 and 100 GeV by utilizing transition radiation (TR) in polypropylene foils and fibres. The innermost pixel layer (also called the B-layer) is located (just outside the beam pipe) at a radius of 50 mm , and provides precision vertexing.

The ATLAS electromagnetic (EM) calorimeter has a fine segmentation in both the lateral ( $\eta \times$ $\phi$ space) and longitudinal directions of the showers [4]. At high energy, most of the EM shower energy is collected in the second layer which has a lateral granularity of $0.025 \times 0.025$ in $\eta \times \phi$ space. The first layer consists of finer-grained strips in the $\eta$-direction (with a coarser granularity in $\phi$ ). These two layers are complemented by a presampler layer with coarse granularity placed in front to correct for energy lost in the material before the calorimeter, and by a back layer behind.

The analysis is based on a data sample collected at $\sqrt{s}=900 \mathrm{GeV}$. The events are triggered during LHC stable beams using the Minimum-Bias-Trigger-Scintillators (MBTS), which cover the pseudorapidity range $2.09<|\eta|<3.84$. Collision candidates are selected using additional timing requirements to provide further rejection against beam backgrounds: either coincident signals from the EM calorimeter end-caps or from the MBTS. Events are required to have good data quality for the tracker, electromagnetic calorimeter and hadronic calorimeter and to have been recorded with the solenoidal field at its nominal value. The data sample obtained consists of 384,186 collision candidates and corresponds to an integrated luminosity of approximately $9 \mu \mathrm{~b}^{-1}$. The Monte Carlo event sample used throughout this note is composed of $10^{7}$ non-diffractive minimum-bias events generated with Pythia, using the ATLAS tune [5], and passed through the full ATLAS simulation and reconstruction software.

## 3 Reconstruction of Converted Photons

The reconstruction of photon conversions uses tracks found by the different track-reconstruction algorithms in ATLAS [6]. The standard inside-out tracking is seeded with hits in the Pixel detector and in the SCT. Tracks found in the silicon detectors are extended outwards into the TRT. The back-tracking

Table 1: Selection criteria for track pairs and fitted vertices in the photon conversion candidate reconstruction.

|  | Silicon-Silicon | Silicon-TRT | TRT-TRT |
| :--- | :---: | :---: | :---: |
| Distance of closest approach | 10 mm | 50 mm | 50 mm |
| $\Delta \cot \theta$ | 0.3 | 0.5 | 0.5 |
| $\Delta \Phi$ | 0.05 | 0.5 | 0.5 |
| $\left(D-R_{1}-R_{2}\right)_{\min }$ | -5 mm | -25 mm | -50 mm |
| $\left(D-R_{1}-R_{2}\right)_{\max }$ | 5 mm | 10 mm | 10 mm |
| $\chi_{\mathrm{vtx}}^{2}$ | 50 | 50 | 50 |

algorithm is seeded from the TRT and the segments found are extended inwards towards the silicon detectors, yielding tracks with silicon hits if the extension has been successful, and stand-alone TRT tracks otherwise.

The photon conversion reconstruction algorithm is described in detail elsewhere [7]. In the following, the basic steps of the algorithm are recalled together with an updated list of selection criteria. The algorithm begins by selecting single tracks with transverse momentum $p_{T}>500 \mathrm{MeV}$ and a significant fraction of high-threshold hits in the TRT, as expected from transition radiation. Photon conversion candidates are then created by pairing oppositely-charged tracks. Three possible combinations of track pairs are considered: two tracks with at least four silicon hits each (Silicon-Silicon track pairs), two stand-alone TRT tracks (TRT-TRT track pairs) and pairs with one track with at least for silicon hits and one stand-alone TRT track (Silicon-TRT track pairs). To reduce the combinatorial background, several selection criteria are applied taking advantage of the specific features expected for secondary vertices from photon conversions. Since the photon is massless, the emerging tracks are almost parallel at the vertex. The tracks are therefore required to be close in space and to have a small opening angle. An additional cut requires the sum of the radii of the helices of the electron and positron tracks, $R_{1}$ and $R_{2}$, to be comparable to the distance between the centers of the two helices, $D$. The selected track pairs are then fitted to a common vertex with the constraint that they be parallel at the vertex. The final set of photon conversion candidates is then selected based on the quality of the vertex fit. The selection criteria for the different track-pair categories are listed in Table 1.

The breakdown of the photon conversions in the different categories of track pairs is given in Table 2. Most of the photon conversion candidates at this stage originate from combinatorial background, which is much lower for pairs containing two precisely measured tracks with silicon hits than for pairs containing TRT stand-alone tracks. Since the determination of the material close to the beam pipe is the most critical for the reconstruction of high-energy photons and electrons, the study focuses in what follows on the 3662 silicon-silicon track-pair candidates.

The agreement between data and Monte Carlo simulation is shown in Fig. 1 where the comparison is presented for a few quantities used to reconstruct photon conversions, shown after the reconstruction cuts, and the transverse momentum of the photon conversion candidates. Given the complexity of the reconstruction of converted photons and the impact of bremsstrahlung of the electrons in the tracker material, the consistency between the data and the simulation for the selection variables is good.

## 4 Estimation of Inner Detector Material

An accurate and high-granularity map of the ID material is necessary for a precise reconstruction of high-energy photons and electrons. The ID material affects both the track trajectories (especially through

Table 2: Breakdown of the number of reconstructed photon conversion candidates built with two tracks with at least four silicon hits each, one track with at least four silicon hits and one stand-alone TRT track and pairs with two stand-alone TRT tracks.

|  | Silicon-Silicon | Silicon-TRT | TRT-TRT | total |
| :---: | :---: | :---: | :---: | :---: |
| Data | $6.7 \% \pm 1.7 \%$ | $31.7 \pm 0.9 \%$ | $61.5 \pm 0.7 \%$ | 54549 |
| Simulation | $10.4 \% \pm 0.3 \%$ | $31.8 \pm 0.2 \%$ | $57.8 \pm 0.1 \%$ | 1364828 |



Figure 1: Comparison between converted photon candidates with at least four silicon hits per track in data and non-diffractive minimum-bias Monte Carlo simulation. Top-left: opening angle in the $R z$ plane between the two tracks $(\Delta(1 / \tan \theta))$; top-right: 3D distance of closest approach between the two tracks; bottom-left: normalised $\chi^{2}$ of the vertex fit; bottom-right: converted photon candidate $p_{T}$. The points show the distribution for all photon conversion candidates in data; the open histograms, the corresponding distributions from the Monte Carlo simulation and the filled histograms show the contribution of true photon conversions as predicted from the Monte Carlo simulation. The distributions are normalized to the same number of photon conversion candidates in data and Monte Carlo simulation.
bremsstrahlung effects) and the electromagnetic shower development (because of the magnetic field and the energy lost in the ID material). This section describes the use of photon conversions as a tool to map precisely the position and amount of material in the tracker.

The radiation length, $\frac{X}{X_{0}}$, of a localized amount of material is related to the fraction of photons, $F_{\text {conv }}$, that convert in it through the relation:

$$
\begin{equation*}
\frac{X}{X_{0}}=-\frac{9}{7} \ln \left(1-F_{\text {conv }}\right) \tag{1}
\end{equation*}
$$

where $F_{\text {conv }}$ can be estimated as

$$
\begin{equation*}
F_{\mathrm{conv}}=\frac{N_{\mathrm{reco}}}{N_{\mathrm{tot}}} \frac{F_{\mathrm{comb}} F_{\mathrm{mis}}}{\varepsilon} \frac{1}{\exp \left(-7 / 9 M_{\mathrm{up}}\right)} \tag{2}
\end{equation*}
$$

In the above, $N_{\text {reco }}$ is the number of reconstructed photon conversions in the slice of material under investigation; $F_{\text {comb }}$ is a correction factor accounting for the contamination from combinatorial background, while $F_{\text {mis }}$ corrects for resolution effects that lead to migration of photon conversion candidates between different detector layers; $N_{\text {tot }}$ is the total number of photons produced at the primary vertex; $\varepsilon$ is the conversion reconstruction and selection efficiency and $M_{\text {up }}$ is the integrated radiation length of the material in front of the slice of material under consideration.

In the following, only tracks with at least four silicon hits are used to reconstruct photon conversions. To further reduce the combinatorial background, each track is required to pass a stricter cut on the TRT particle identification and the normalised $\chi^{2}$ is required to be smaller than 5 . The requirement on the TRT particle identification is based on a likelihood ratio constructed from Monte Carlo simulation of electron and pion tracks and calibrated on test-beam measurements.

To quantify the agreement between data and Monte Carlo simulation, the number of converted photons measured from data is compared to the number expected from Monte Carlo simulation in different regions of the inner detector. Due to the limited statistics, even a coarse comparison is only possible within the volume delimited by the first layer of the SCT.
The number of photon conversions reconstructed within $R<340 \mathrm{~mm}$ is 244 in a total of 384,186 events; the corresponding number for the $10^{7}$ events Monte Carlo sample is 9218 , which corresponds to 354 photon conversions for the equivalent data statistics.

The number of photon conversions per event is not well reproduced by the Monte Carlo simulation, which can be attributed to the simulation of the photon production or the overall reconstruction efficiency. Neither of these is the focus of this study. For this reason, in what follows, the total number of photon conversions in Monte Carlo simulation are normalized to total number of photon conversions reconstructed in data.

In Tables 3 and 4, the comparison between the number of photon conversions reconstructed in data and simulation are compared for different volumes. The model used for the simulation appears to be correctly describing the detector.

The results for the distributions of the photon conversion vertices in the radial direction and in $\eta$ (defined with respect to the centre of the detector) in Fig. 2 show, albeit with limited statistics, a good match between the measured material distribution and the Monte Carlo model. The observed asymmetry in the $\eta$ distribution can be attributed to an $\eta$-asymmetry in the number of inoperable Pixel detector modules. The effect is well-modeled by the simulation.

Using Eqs. 1 and 2 it is possible to extract the amount of material in any volume of the detector. The remaining combinatorial background and the migration of reconstructed converted photon candidates between different silicon layers due to mis-reconstruction of the vertex and the efficiencies are estimated using the Monte Carlo simulation. The efficiency (quoted in Tab. 5) represents the reconstruction and selection efficiency after applying the cuts used to map the tracker material. The efficiency can be broken

Table 3: Comparison of the number of photon conversions reconstructed in data and Monte Carlo simulation for different volumes in the ID. The values are integrated within the limits shown in each row. The distributions are normalized to the same number of photon conversion candidates in data and Monte Carlo simulation.

|  | $\phi$ | Data | MC | Data/MC |
| :---: | :---: | :---: | :---: | :---: |
| $R<500 \mathrm{~mm}$ | $-\pi \leq \phi<-\pi / 2$ | 67 | 61 | $1.09 \pm 0.13$ |
|  | $-\pi / 2 \leq \phi<0$ | 59 | 62 | $0.95 \pm 0.12$ |
|  | $0 \leq \phi<\pi / 2$ | 74 | 68 | $1.09 \pm 0.13$ |
|  | $\pi / 2 \leq \phi \leq \pi$ | 53 | 62 | $0.85 \pm 0.12$ |
| $R<340 \mathrm{~mm}$ | $-\pi \leq \phi<-\pi / 2$ | 65 | 58 | $1.12 \pm 0.14$ |
|  | $-\pi / 2 \leq \phi<0$ | 55 | 59 | $0.93 \pm 0.13$ |
|  | $0 \leq \phi<\pi / 2$ | 73 | 65 | $1.12 \pm 0.13$ |
|  | $\pi / 2 \leq \phi \leq \pi$ | 51 | 60 | $0.85 \pm 0.12$ |
| $R<240 \mathrm{~mm}$ | $-\pi \leq \phi<-\pi / 2$ | 57 | 51 | $1.12 \pm 0.15$ |
|  | $-\pi / 2 \leq \phi<0$ | 46 | 52 | $0.88 \pm 0.13$ |
|  | $0 \leq \phi<\pi / 2$ | 60 | 58 | $1.03 \pm 0.13$ |
|  | $\pi / 2 \leq \phi \leq \pi$ | 46 | 52 | $0.88 \pm 0.13$ |

Table 4: The first half of the table shows the number of photon conversions reconstructed in data on the beam pipe and on the first four silicon layers; the second half shows the ratio with respect to the Monte Carlo simulation. The values are integrated over the entire azimuthal angle and over the $\eta$ ranges specified in each column.

|  | $\|\eta\|<2.5$ | $\|\eta\|<0.7$ | $0.7<\|\eta\|<1.4$ | $1.4<\|\eta\|<2.5$ |
| :--- | :---: | :---: | :---: | :---: |
| Beam pipe | 9 | 1 | 3 | 5 |
| Pixel B-layer | 46 | 5 | 17 | 24 |
| Pixel layer 1 | 65 | 16 | 17 | 32 |
| Pixel layer 2 | 55 | 10 | 15 | 30 |
| SCT layer 1 | 25 | 9 | 5 | 11 |
| Beam pipe | $0.90_{-0.29}^{+0.41}$ | $0.50_{-0.41}^{+1.1}$ | $1.00_{-0.54}^{+0.97}$ | $0.83_{-0.36}^{+0.85}$ |
| Pixel B-layer | $0.85 \pm 0.13$ | $0.38_{-0.17}^{+0.26}$ | $1.13 \pm 0.27$ | $0.89 \pm 0.18$ |
| Pixel layer 1 | $1.16 \pm 0.14$ | $1.23 \pm 0.31$ | $1.06 \pm 0.26$ | $1.14 \pm 0.20$ |
| Pixel layer 2 | $0.96 \pm 0.13$ | $0.83_{-0.26}^{+0.36}$ | $1.00 \pm 0.26$ | $1.03 \pm 0.19$ |
| SCT layer 1 | $1.14 \pm 0.23$ | $1.80_{-0.59}^{+0.82}$ | $0.83_{-0.36}^{+0.85}$ | $1.00_{-0.30}^{+0.40}$ |



Figure 2: Distribution of photon conversion candidate radius $R$ integrated over all $\eta$ (top-left), $\eta$ integrated over all $R$ (top-right), and distribution of photon conversion candidate radius in $|\eta|<0.7$ (bottomleft) and $|\eta|>1.4$ (bottom-right). The points show the distribution for all photon conversion candidates in data; the open histograms, the corresponding distributions from the Monte Carlo simulation and the filled histograms show the contribution of true photon conversions as predicted from the Monte Carlo simulation. The contribution from the Dalitz decays of neutral mesons is shown in the radial distribution integrated over all $\eta$. The radial distributions for the separate $\eta$ regions are shown for $R>24 \mathrm{~mm}$, which corresponds to about six times the resolution of the vertex radial position, to ensure a good reconstruction of the $\eta$ of the vertex. The distributions are normalized to the same number of photon conversion candidates in data and Monte Carlo simulation.

Table 5: $N_{\text {reco }}$ is the number of reconstructed photon conversions. $F_{\text {comb }}, F_{\text {mis }}, \varepsilon$ are correction factors extracted from Monte Carlo simulation to quantify the purity of the converted photon sample, the misreconstruction of the vertex position (how often a photon conversion is assigned to the wrong volume) and the reconstruction and selection efficiencies. $\frac{X}{X_{0}}{ }_{\text {data }}, \frac{X}{X_{0}} \mathrm{MC}$ and $\frac{X}{X_{0}}$ data $/ \frac{X}{X_{0}} \mathrm{MC}$ represent the radiation length of the material in the different volumes estimated from data and Monte Carlo simulation and their ratios. The normalization to the number of reconstructed converted photons at the beam pipe introduces an additional uncertainty of $30 \%$ on $\frac{X}{X_{0}}$ data , which has been taken into account in the ratio of the radiation lengths in data and Monte Carlo simulation.

|  | $N_{\text {reco }}$ | $F_{\text {comb }}$ | $F_{\text {mis }}$ | $\varepsilon$ | $\frac{X}{X_{0}}$ data | $\frac{X}{X_{0}}$ MC | $\frac{X}{X_{0}}{ }_{\text {data }} / \frac{X}{X_{0}} \mathrm{MC}$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Beam pipe | 9 | 0.91 | 0.99 | 0.033 | 0.00655 | 0.00655 |  |
| Pixel B-layer | 46 | 0.97 | 0.97 | 0.038 | $0.031 \pm 0.005$ | 0.032 | $0.98 \pm 0.36$ |
| Pixel layer 1 | 65 | 0.98 | 0.95 | 0.046 | $0.036 \pm 0.005$ | 0.027 | $1.34 \pm 0.48$ |
| Pixel layer 2 | 55 | 0.97 | 0.88 | 0.052 | $0.025 \pm 0.004$ | 0.023 | $1.12 \pm 0.41$ |
| SCT layer 1 | 25 | 0.99 | 0.97 | 0.034 | $0.021 \pm 0.004$ | 0.016 | $1.31 \pm 0.52$ |

down into the different reconstruction and selection steps: the single track reconstruction efficiency is about $65 \%$; the two-track efficiency is about $50 \%$; the conversion finding efficiency (i.e. after the constrained vertex fit) about $35 \%$ and the final selection to achieve the high purity photon conversion sample brings the efficiency to about $5 \%$. At each step the efficiency is calculated using as numerator the number of reconstructed tracks (photon conversions) and as denominator the number of truth tracks (photon conversions) within the fiducial volume defined by the acceptance of the tracker $(|\eta|<2.5$, conversion radius $R<800 \mathrm{~mm}$ ) or a given detector layer, and requiring the transverse momenta of the tracks above 500 MeV . To remove the dependence on the unknown number of photons produced at the primary vertex (mostly from the decay of neutral mesons), the reconstructed number of photon conversions in a given slice of the detector is normalized to the number of photon conversions in a reference volume. The beam pipe has been chosen as the reference because of its well-known material composition and because of its location upstream of the rest of the tracker. This method, which has been successfully tested on Monte Carlo simulation and demonstrated in the ATLAS Combined Test Beam [8], is applied here to collision data. The agreement between data and Monte Carlo simulation is presented in Tab. 5.
The tiny number of conversions on the beam pipe is presently the main limitation on the accuracy of this method. With larger data samples, the dominating systematic uncertainty on the material estimation will come from the determination of the photon conversion reconstruction efficiency.

## 5 Dalitz Decays

The neutral mesons produced at the primary vertex can decay to a pair of photons or through a Dalitz process, e.g. $\pi^{0} \rightarrow e^{+} e^{-} \gamma$. The branching ratios for the $\pi^{0}$, the neutral meson which is most abundantly produced in collisions, are very precisely measured: $\operatorname{BR}\left(\pi^{0} \rightarrow \gamma \gamma\right)=(98.798 \pm 0.032) \%$ and $\operatorname{BR}\left(\pi^{0} \rightarrow\right.$ $\left.e^{+} e^{-} \gamma\right)=(1.198 \pm 0.032) \%$. The ratio of photon conversions in a given volume to the number of Dalitz decays allows the setting of very stringent constraints on the amount of material in it. In particular, this can be used to constrain the amount of material in the beam pipe where the reconstruction efficiency is expected to be the same as at the primary vertex.

The reconstructed electron-positron pairs originating from the Dalitz decays of neutral mesons appear in Fig. 3 as conversion candidates occurring at the primary vertex. In the present data sample, nine photon


Figure 3: Distribution of $\pi^{0}$ Dalitz decays and photon conversion radius in Fig. 2, shown in more detail.
conversion candidates on the beam pipe and five Dalitz decays have been reconstructed. The two types of candidates are separated according to the reconstructed radial position of the vertex: Dalitz decay candidates are required to have a radial position of less than 20 mm from the beam spot, candidates for conversions on the beam pipe to have a radial position between 20 mm and 40 mm . The ratio of beam pipe photon conversions to Dalitz decays of $1.8 \pm 1$ is in agreement with the ratio expected from Monte Carlo simulation, $2.04 \pm 0.19$.

## 6 Reconstruction of $\pi^{0}$ Mesons Using Converted Photons

The reconstruction of $\pi^{0}$ mesons from two unconverted photons in the ATLAS detector has been extensively studied [10]. Here the study of $\pi^{0}$ reconstruction using one converted and one unconverted photon candidate is presented.

In addition to the converted photon candidates reconstructed in the tracker, unconverted photon candidates are reconstructed from clusters in the electromagnetic calorimeter. The clusters are built by a topological algorithm, which starts with a seed cell where the deposited energy is larger than four standard deviations above the expected noise and iteratively adds the neighboring cells passing certain threshold criteria. To suppress backgrounds from charged particles, clusters with a matching silicon or stand-alone TRT track are vetoed. In particular, this includes tracks that are used for the reconstruction of photon conversion candidates, which reduces the combinatorial background. The track-cluster matching is performed by extrapolating a given track from its last measurement in the tracker to the second layer of the electromagnetic calorimeter and by comparing the angular distance of the extrapolated track position to the angular position of the cluster. A wide window is used for the matching: $\Delta \phi<0.5(0.3)$ on the side where losses from bremsstrahlung are (are not) expected and for tracks with silicon hits $\Delta \eta<0.1$; for tracks without silicon hits, the matching in $\eta$ is relaxed, such that only matching of detector regions (barrel vs endcaps) is required. In addition, a transverse energy of the cluster greater than 300 MeV is required.

All reconstructed photon conversion candidates with at least four silicon hits per track are used in this analysis. To reduce combinatorial background, the two-photon candidates are required to be in the same hemisphere of the detector.


Figure 4: Invariant mass distribution of one converted and one unconverted photon as measured on data (points) and Monte Carlo simulation (histogram).

The $\gamma e^{+} e^{-}$-invariant-mass distribution for $p_{T}^{\gamma e^{+} e^{-}}>900 \mathrm{MeV}$ is shown in Fig. 4. The $\pi^{0}$ peak can be clearly observed. No energy corrections are applied to the reconstructed clusters, which accounts for the majority of the shift of the reconstructed $\pi^{0}$ mass compared to the true $\pi^{0}$ mass. This effect is well reproduced by the simulation, as is the width of the $\pi^{0}$ peak and the shape of the combinatorial background.

## 7 Conclusion

The analysis of the photon conversions reconstructed in the $\sqrt{s}=900 \mathrm{GeV}$ run in 2009 demonstrates the excellent performance of the conversion reconstruction algorithm. The spatial distributions of the photon conversion vertices show, albeit with low statistics, that the Monte Carlo model of the tracker represents the installed detector well. The number of reconstructed neutral meson Dalitz decays matches the one expected from Monte Carlo simulations. The $\pi^{0}$ reconstruction with one converted and one unconverted photon has been performed and agrees with expectations, demonstrating the ATLAS capability to combine both calorimeter and tracker information.

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# Observation of $W \rightarrow \ell v$ and $Z \rightarrow \ell \ell$ production in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

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#### Abstract

This note describes an observation by the ATLAS experiment of $57 W \rightarrow \ell v$ candidates and three $Z \rightarrow \ell \ell$ candidates, where $\ell=e, \mu$, produced in $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions at the LHC. These results correspond to total integrated luminosities of $6.7 \mathrm{nb}^{-1}$ for the $W \rightarrow e v$ and $Z \rightarrow e e$ channels, and $6.4 \mathrm{nb}^{-1}$ and $7.9 \mathrm{nb}^{-1}$ for the $W \rightarrow \mu \nu$ and $Z \rightarrow \mu \mu$ channels, respectively. The number of events observed is consistent with the expectations.


## 1 Introduction

The experimental study of the electroweak gauge bosons has a history of about thirty years. The $W$ and the $Z$ particles were initially discovered and measured at the CERN proton-antiproton collider in 1983 [1, 2, 3, 4]. During the early 1990's, the $Z$ properties were measured in great detail at the high energy $e^{+} e^{-}$colliders LEP and SLC [5]. In the second half of that decade, an energy increase of LEP allowed to measure $W$ bosons produced in pairs. The Tevatron proton-antiproton collider has been accumulating $W$ and $Z$ events over the last twenty years. The results of these programmes include highprecision measurements of the $W$ and $Z$ mass, width, and couplings, as well as detailed information on their production in proton-antiproton collisions and corresponding constraints on the proton parton density functions [6]. The current uncertainties on the intrinsic properties of the $W$ boson are about ten times larger than their $Z$ counterparts [7].

The $W$ and $Z$ bosons are expected to be produced abundantly at the Large Hadron Collider (LHC) [8], and for the first time in proton-proton collisions. This significant dataset and the high LHC energy will allow for detailed measurements of their production properties at a previously unexplored energy scale. These conditions, together with the particular nature of the collisions, will provide new insights on the proton properties, tests of perturbative QCD calculations, and ultimately a precise determination of the mass of the $W$ boson [9]. In this process, the well-known properties of the $Z$ boson will provide significant constraints on the determination of the performance of the collider experiments at the LHC; its known mass, width and leptonic decays can be exploited to measure precisely the detector energy and momentum scale, resolution, as well as lepton identification and trigger efficiencies.

The critical first step in making such precision measurements is an observation of $W$ and $Z$ production at the LHC. This note details an observation by the ATLAS [10] experiment of $17 \mathrm{~W} \rightarrow e v$ and 40 $W \rightarrow \mu \nu$ candidates produced from the $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions of the LHC, resulting from total integrated luminosities of $6.7 \mathrm{nb}^{-1}$ and $6.4 \mathrm{nb}^{-1}$ in the electron and muon channels, respectively. One $Z \rightarrow e e$ and two $Z \rightarrow \mu \mu$ candidates were also observed with data corresponding to integrated luminosities of $6.7 \mathrm{nb}^{-1}$ and $7.9 \mathrm{nb}^{-1}$, respectively. These data were collected over a seven-week period from March to May 2010. The uncertainty on the luminosity determination is on the order of $20 \%$.

In this note, the nominal interaction point is defined as the origin of the coordinate system, while the beam direction defines the $z$-axis and the $x-y$ plane is transverse to the beam direction. The positive $x$-axis is defined as pointing from the interaction point to the centre of the LHC ring and the positive $y$-axis is defined as pointing upwards. The azimuthal angle $\phi$ is measured around the beam axis and the polar angle $\theta$ is the angle from the beam axis. The pseudorapidity is defined as $\eta=-\ln \tan (\theta / 2)$. The transverse momentum $p_{\mathrm{T}}$, the transverse energy $E_{\mathrm{T}}$, and the transverse missing energy $E_{\mathrm{T}}^{\text {miss }}$ are defined in the $x-y$ plane. The distance $\Delta R$ in the $\eta-\phi$ space is defined as $\Delta R=\sqrt{\Delta \eta^{2}+\Delta \phi^{2}}$.

## 2 The ATLAS detector

The ATLAS detector [10] at the LHC comprises of a thin superconducting solenoid surrounding the inner-detector cavity and three large superconducting toroids arranged with an eight-fold azimuthal coil symmetry placed around the calorimeters, forming the basis of the muon spectrometer.

The Inner-Detector (ID) system is immersed in a 2 T axial field and provides tracking information on charged particles in a pseudorapidity range matched by the precision measurements of the electromagnetic calorimeter. The silicon tracking detectors, pixel and silicon microstrip (SCT), cover the pseudorapidity range $|\eta|<2.5$. The highest granularity is achieved around the vertex region using the pixel detectors. Typically three pixel layers are crossed by each track. For the SCT, eight strip layers (providing four space points) are crossed by each track in the barrel region. A large number of hits (typically 36 per track) is provided by the Transition Radiation Tracker (TRT), which enables track-following up
to $|\eta|=$ 2.0. The electron identification information is provided by the detection of transition radiation in the xenon-based gas mixture of the TRT straw tubes.

The calorimeter system covers the pseudorapidity range $|\eta|<4.9$, using a variety of detector technologies. The lead-liquid argon (LAr) electromagnetic (EM) calorimeter is divided into a barrel part ( $|\eta|<1.475$ ) and two end-cap components ( $1.375<|\eta|<3.2$ ). Over the region devoted to precision physics ( $|\eta|<2.5$ ), the EM calorimeter is segmented in three sections in depth. The remaining portion of the EM calorimeter, known as the end-cap inner wheel, is segmented in two sections in depth and has a coarser lateral granularity than for the rest of the acceptance. In the region of $|\eta|<1.8$, a thin LAr presampler detector is used to correct for the energy lost by electrons, positrons, and photons upstream of the calorimeter. The hadronic tile calorimeter is placed directly outside the EM calorimeter envelope. This steel/scintillating-tile detector consists of a barrel covering the region $|\eta|<1.0$, and two extended barrels in the range $0.8<|\eta|<1.7$. The copper-LAr Hadronic End-cap Calorimeter (HEC) consists of two independent wheels per end-cap $(1.5<|\eta|<3.2)$, located directly behind the end-cap electromagnetic calorimeter. The Forward Calorimeter ( FCal ) consists of three modules in each end-cap: the first, made of copper-LAr, is optimised for electromagnetic measurements, while the other two, made of tungsten-LAr, measure primarily the energy of hadronic interactions.

The muon spectrometer is based on the magnetic deflection of muon tracks in the large superconducting air-core toroid magnets, instrumented with separate trigger and high-precision tracking chambers. A system of three large air-core toroids, a barrel and two end-caps, generates the magnetic field for the muon spectrometer in the pseudorapidity range of $|\eta|<2.7$. In the barrel region, tracks are measured in chambers arranged in three cylindrical layers around the beam axis; in the transition and end-cap regions, the chambers are installed in planes perpendicular to the beam, also in three layers. Over most of the $\eta$-range, a precision measurement of the track coordinates in the principal bending direction of the magnetic field is provided by Monitored Drift Tubes (MDT's). At large pseudorapidities, Cathode Strip Chambers (CSC's) with higher granularity are used in the innermost plane over $2<|\eta|<2.7$, to withstand the demanding rate and background conditions expected with the LHC operation at the nominal luminosity and centre-of-mass energy. The trigger system which covers the pseudorapidity range $|\eta|<2.4$ consists of Resistive Plate Chambers (RPC's) in the barrel ( $|\eta|<1.05$ ) and Thin Gap Chambers (TGC's) in the end-cap regions.

The first-level (L1) trigger system uses a subset of the total detector information to make a decision on whether or not to process an event. Details about L1 calorimeter and muon trigger systems used in the analysis of the $W$ and $Z$ candidates are provided in Section 5.

## $3 W, Z$ processes and sources of background

The results presented in this note are compared to expectations based on Monte Carlo simulations. The signal and background samples used in this note were generated at $\sqrt{s}=7 \mathrm{TeV}$ with PYTHIA [11] using MRST LO [12] parton distribution functions (PDF), then simulated with GEANT4 [13] and fully reconstructed. These samples are summarised in Table 1.

The $W$ and $Z$ production cross sections times their respective $W \rightarrow \ell \nu$ and $Z / \gamma^{*} \rightarrow \ell \ell$ decay branching ratios used in this study are calculated at next-to-next-to-leading order (NNLO) in QCD corrections using the FEWZ program [14] with the MSTW2008 parton distribution function set [15]. The dilepton invariant mass of the $Z / \gamma^{*} \rightarrow \ell \ell$ process is chosen to be greater than 60 GeV . These values are:

$$
\begin{equation*}
\sigma_{W \rightarrow \ell v}^{N N L O}=10.45 \mathrm{nb} \text { and } \sigma_{Z / \gamma^{*} \rightarrow \ell \ell}^{N N L O}=0.989 \mathrm{nb} \tag{1}
\end{equation*}
$$

The estimated uncertainties for both cross sections coming from the factorization and renormalization scales as well as the parton distribution functions are expected to be approximately $3 \%[16,17,18]$.

| Physics process | Cross section (nb) $[\times \mathrm{BR}]$ | Luminosity $\left(\mathrm{nb}^{-1}\right)$ |
| :--- | :---: | :---: |
| $\mathrm{W} \rightarrow e v$ | 10.45 | $6.7 \times 10^{5}$ |
| $\mathrm{~W} \rightarrow \mu \nu$ | 10.45 | $6.7 \times 10^{5}$ |
| $\mathrm{~W} \rightarrow \tau \nu \rightarrow \ell \nu v(\ell=\mu, e)$ | 3.68 | $3.1 \times 10^{5}$ |
| $\mathrm{Z} \rightarrow e e\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.989 | $4.8 \times 10^{6}$ |
| $\mathrm{Z} \rightarrow \mu \mu\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.989 | $5.1 \times 10^{6}$ |
| $\mathrm{Z} \rightarrow \tau \tau\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.989 | $2.0 \times 10^{6}$ |
| $t \bar{\epsilon}$ | 0.16 | $2.5 \times 10^{6}$ |
| Dijet (electron channel, $\left.\hat{p}_{T}>15 \mathrm{GeV}\right)$ | $1.15 \times 10^{6}$ | 100 |
| Dijet (muon channel, $\left.8<\hat{p}_{\mathrm{T}}<17 \mathrm{GeV}\right)$ | $9.86 \times 10^{6}$ | 0.05 |
| Dijet (muon channel, $\left.17<\hat{p}_{\mathrm{T}}<35 \mathrm{GeV}\right)$ | $6.78 \times 10^{5}$ | 0.74 |
| Dijet (muon channel, $\left.35<\hat{p}_{\mathrm{T}}<70 \mathrm{GeV}\right)$ | $4.10 \times 10^{4}$ | 12.20 |
| Dijet (muon channel, $\left.70<\hat{p}_{\mathrm{T}}<140 \mathrm{GeV}\right)$ | $2.20 \times 10^{3}$ | 227.74 |
| Dijet (muon channel, $\left.140<\hat{p}_{\mathrm{T}}<280 \mathrm{GeV}\right)$ | $0.88 \times 10^{2}$ | $5.70 \times 10^{3}$ |
| Dijet (muon channel, $280<\hat{p}_{\mathrm{T}}<1120 \mathrm{GeV}$ ) | 2.35 | $2.13 \times 10^{5}$ |

Table 1: Signal and background Monte Carlo samples used in the electron and muon channel analyses, including the production cross section (multiplied by the relevant branching ratios (BR)) and the integrated luminosity of the samples. The variable $\hat{p}_{T}$ is the transverse momentum of the partons involved in the hard scatter. $W$ and $Z$ cross sections are given at NNLO, the $t \bar{t}$ cross section is given at next-to-leading order (plus next-to-next-to-leading log), and the dijet cross sections are given at leading order.

The background contributions, expected primarily from jet production via QCD processes, have significant components from semi-leptonic decays of heavy quarks, hadrons misidentified as leptons, and in the case of the electron channel, electrons from conversions. For both the electron and muon channels, these sources of background have been obtained from dijet samples.

In the case of the $W$ analysis, $W$ events decaying into $\tau$-leptons with subsequent leptonic $\tau$ decays are also expected to contribute in both channels. Contributions from $Z \rightarrow \mu \mu$ decays are significant in the muon channel. Due to the $\eta$ coverage of the muon system, this type of decay is more likely to generate $E_{\mathrm{T}}^{\text {miss }}$ in the muon channel than $Z \rightarrow e e$ decays in the electron channel. The muon channel additionally takes into account contributions from $Z \rightarrow \tau \tau$ decays and from $t \bar{t}$ events involving at least one semi-leptonic decay, though these contributions are small.

## 4 Object reconstruction

### 4.1 Electrons

The ATLAS standard electron/photon reconstruction and identification algorithm [19] is designed to provide various levels of background rejection optimised for high identification efficiencies for transverse energy $E_{\mathrm{T}}>20 \mathrm{GeV}$, over the full acceptance of the inner-detector system. Electron reconstruction begins with a seed cluster of energy of $E_{\mathrm{T}}>2.5 \mathrm{GeV}$ in the second layer of the electromagnetic calorimeter. This cluster of size $\Delta \eta \times \Delta \phi=0.075 \times 0.125$ is selected by a sliding window algorithm. A matching track, extrapolated to the middle EM calorimeter layer, is searched for in a broad window of $\Delta \eta \times \Delta \phi=0.05 \times 0.1$ amongst all reconstructed tracks with $p_{\mathrm{T}}>0.5 \mathrm{GeV}$. The closest-matched track to this layer's cluster barycentre is kept as that belonging to the electron candidate. The final electron candidates have cluster sizes of $\Delta \eta \times \Delta \phi=0.075 \times 0.175$ in the barrel calorimeter and $0.125 \times 0.125$ in the end-cap. The total
transverse energy of these clusters is the $E_{\mathrm{T}}$ used in this analysis.
The baseline electron identification selections [19] are based on criteria using calorimeter and tracker information and have been optimised in 10 bins in $\eta$ and 11 bins in $E_{\mathrm{T}}$. Three reference sets of requirements (loose, medium, and tight) have been chosen, providing progressively stronger jet rejection at the expense of some identification efficiency loss. Each set adds additional constraints to the previous requirements:

- Loose: this basic selection uses EM shower shape information from the second layer of the EM calorimeter (lateral shower containment and shower width) and energy leakage into the hadronic calorimeters as discriminant variables. This set of requirements provides high and uniform identification efficiency but a low background rejection;
- Medium: this selection provides additional hadronic rejection by evaluating the energy deposit patterns in the first layer of the EM calorimeter (the shower width and the ratio of the energy difference associated with the largest and second largest energy deposit over the sum of these energies), track quality variables (number of hits in the pixel and silicon trackers, the transverse impact parameter) and a cluster-track matching variable ( $\eta$ between the cluster and the track extrapolated to the first layer of the EM calorimeter)
- Tight: this selection further rejects charged hadrons and secondary electrons from conversions by fully exploiting the electron identification potential of the ATLAS detector. It makes requirements on the ratio of cluster energy to track momentum, on the number of hits in the TRT, and on the ratio of high-threshold to the total number of hits in the TRT. Electrons from conversions are rejected by requiring at least one hit in the first layer of the pixel detector. A conversion-flagging algorithm is also used to further reduce this contribution. The impact-parameter requirement applied in the medium selection is further tightened at this level.

Using $Z \rightarrow e e$ signal and QCD dijet Monte Carlo samples for electrons with $E_{T}>20 \mathrm{GeV}$ within the range $|\eta|<2.47$ and excluding the transition region between the barrel and end-cap calorimeters ( $1.37<|\eta|<1.52$ ), the expected identification efficiencies are estimated to be $94 \%, 90 \%$, and $72 \%$ with respective rejection factors against background jets with true $E_{\mathrm{T}}>20 \mathrm{GeV}$ of 1100,6800 , and 92000 for loose, medium, and tight electron identification, respectively [19].

### 4.2 Muons

The ATLAS muon identification and reconstruction algorithms take advantage of the multiple subdetector technologies which provide complementary approaches and cover pseudorapidities up to 2.7 over a wide $p_{\mathrm{T}}$ range [9].

The stand-alone muon reconstruction is based entirely on muon-spectrometer information, independently of whether or not this track is also reconstructed in the inner detector. The muon reconstruction is initiated locally in a muon chamber by the search for straight line track segments in the bending plane. Hits in the precision chambers are used and the segment candidates are requested to point to the centre of ATLAS. The hit coordinate $\phi$ in the non-bending plane measured by the trigger detectors is associated to the segment when available. A minimum of two track segments in different muon stations are combined to form a muon track candidate using three-dimensional tracking in the magnetic field. The track parameters $\left(p_{\mathrm{T}}, \eta, \phi\right.$, distance of closest approach to the primary vertex along the beam axis and transverse to it) are obtained from the muon spectrometer track fit and are extrapolated to the interaction point taking into account both multiple scattering and energy loss in the calorimeters. For the latter, the reconstruction utilises either a parameterisation or actual measurements of calorimeter energy losses, together with parameterisation of energy loss in the inert material. The typical muon energy loss in the calorimeters is

3 GeV . The stand-alone muon reconstruction algorithms use the least-squares formalism to fit tracks in the muon spectrometer and most material effects are directly integrated into the $\chi^{2}$ function.

The combined muon reconstruction associates the stand-alone muon spectrometer tracks to an innerdetector track, that measures the bending of the muon within the solenoid, using the pixel, SCT and TRT detectors. The association between the stand-alone and inner-detector tracks is performed using a $\chi^{2}$, defined from the difference between the respective track parameters weighted by their combined covariance matrices. The parameters are evaluated at the point of minimum approach to the beam axis. The combined track parameters are derived either from a statistical combination of the two tracks or from a refit of the full track. To validate the results presented in this note, these two independent reconstruction chains were exercised, leading to a good agreement. The results presented here are based on the one which relies on the statistical combination of muon-spectrometer and inner-detector measurements.

The reconstruction and identification efficiencies for muons with $p_{\mathrm{T}}>10 \mathrm{GeV}$ as extracted from $W$ and $Z$ signal Monte Carlo samples is estimated to be $94 \%$ [9]. The availability of muons with energies up to 100 GeV energy in cosmic rays has enabled the commissioning of the muon identification system. Results from these studies indicate that the performance is in agreement with Monte Carlo expectation in this entire energy range. The tracking resolution has been measured to be better than $5 \%$ and the muon detection efficiency is in reasonable agreement with the values measured in simulated events. Detailed studies in collision data are underway but are currently limited by the number of high- $p_{\mathrm{T}}$ muons collected so far.

### 4.3 Transverse missing energy

The transverse missing energy ( $E_{\mathrm{T}}^{\text {miss }}$ ) reconstruction used in the electron channel is currently only based on calorimeter information. This relies on a cell-based algorithm which sums the electromagnetic-scale energy deposits of calorimeter cells inside three-dimensional topological clusters [20]. The EM scale is the energy deposited in the calorimeter calculated under the assumption that all processes are purely electromagnetic in nature. No corrections for the different calorimeter response to hadrons and electrons or photons nor for dead material losses are applied. These topological clusters are built around energy $E>4 \sigma_{\text {noise }}$ seeds, where $\sigma_{\text {noise }}$ is the Gaussian width of the cell energy distribution in randomly triggered events, by iteratively gathering neighbouring cells with $E>2 \sigma_{\text {noise }}$ and, in a final step, by adding all direct neighbours of these accumulated secondary cells. The $x$ - and $y$-components of the calorimeter $E_{\mathrm{T}}^{\text {miss }}$ term are calculated by summing over the transverse energies measured in these topological cluster cells $i$ :

$$
\begin{equation*}
E_{x, y}^{\text {Electron,miss }}=E_{x, y}^{\text {Calo,miss }}=-\sum_{i} E_{x, y} . \tag{2}
\end{equation*}
$$

The $E_{\mathrm{T}}^{\text {miss }}$ used in the muon channel is calculated from the reconstructed momenta of muons measured in the range of pseudorapidity $|\eta|<2.7$ and the calorimeter term as given in Eq. 2:

$$
\begin{equation*}
E_{x, y}^{\text {Muon,miss }}=-\left(\sum_{\text {Muons }} E_{x, y}+\sum_{i} E_{x, y}\right)=-\left(\sum_{\text {isolated }} p_{x, y}+\sum_{n o n-\text { isolated }} p_{x, y}\right)+E_{x, y}^{\text {Calo,miss }}, \tag{3}
\end{equation*}
$$

where non-isolated muons are those within a distance $\Delta R \leq 0.3$ of another jet in the event. The $p_{\mathrm{T}}$ of an isolated muon is determined from the combined measurement of the inner detector and muon spectrometer as explained in Section 4.2. The energy lost by an isolated muon in the calorimeters is not added to the calorimeter term. For a non-isolated muon, the energy lost in the calorimeter cannot be separated from the nearby jet energy. The muon spectrometer measurement of the muon momentum after energy loss in the calorimeter is therefore used unless there is a significant mis-match between the spectrometer and combined measurements, in which case the combined measurement minus the parameterised energy loss in the calorimeter is used. For higher values of the pseudorapidity outside the
fiducial volume of the inner detector $(2.5<|\eta|<2.7)$, there is no matched track requirement and the muon spectrometer stand-alone measurement is used instead.

In both the electron and muon cases, the $E_{T}^{m i s s}$ is defined as:

$$
\begin{equation*}
E_{\mathrm{T}}^{m i s s}=\sqrt{\left(E_{x}^{m i s s}\right)^{2}+\left(E_{y}^{m i s s}\right)^{2}} . \tag{4}
\end{equation*}
$$

The performance of the $E_{\mathrm{T}}^{\mathrm{miss}}$ reconstruction in minimum-bias data is described in Ref. [21].

## 5 Event selection and preparation

### 5.1 Event selection

The results presented in this note were collected over a seven-week period, from March to May 2010. From all data taken at a centre-of-mass energy of 7 TeV and for which the LHC declared stable beams, only those with the detector high voltage in nominal condition are selected. In addition, while the electron channel analysis requires the solenoid to be on, the muon channel analysis needs both solenoid and toroid at nominal field. Finally, both leptonic channels require that all of the sub-detectors are operational such that the response and main criteria needed for particle identification as well as energy and momentum computations do not deviate significantly from their expected behaviour. These basic dataquality requirements resulted in total integrated luminosities of $6.7 \mathrm{nb}^{-1}$ for the $W \rightarrow e v$ and $Z \rightarrow e e$ channels, and $6.4 \mathrm{nb}^{-1}$ and $7.9 \mathrm{nb}^{-1}$ for the $W \rightarrow \mu \nu$ and $Z \rightarrow \mu \mu$ channels, respectively. While the $W \rightarrow \mu \nu$ analysis requires calorimeter information to calculate the $E_{\mathrm{T}}^{\mathrm{miss}}$, no calorimeter information is required for the $Z \rightarrow \mu \mu$ channel. This is the reason why they do not have the same integrated luminosity. The uncertainty on the luminosity determination is on the order of $20 \%$, though the relative luminosity between the various channels is known to a much higher precision.

Events are selected with the hardware-based L1 trigger. The L1 calorimeter trigger selects photons and electrons within $|\eta|<2.5$ using calorimeter information with the reduced granularity of trigger towers of dimension $\Delta \eta \times \Delta \phi=0.1 \times 0.1$. The calorimeter trigger used in this analysis accepts electron and photon candidates if the signal from a cluster of trigger towers is above two trigger counts, where one count corresponds to approximately 1 GeV . The L1 muon trigger searches for patterns of hits within $|\eta|<2.4$ consistent with high- $p_{\mathrm{T}}$ muons originating from the interaction region. The trigger logic is based on three trigger stations. The algorithm requires a coincidence of hits in the different trigger stations within a road, which tracks the path of a muon from the interaction point through the detector. The width of the road is related to the $p_{\mathrm{T}}$ threshold to be applied. The muon trigger used in this analysis corresponds to the lowest $p_{\mathrm{T}}$ threshold trigger which has a fully-opened road with a two-station coincidence. As a result of these trigger decisions, $1.2 \times 10^{7}$ and $2.8 \times 10^{5}$ events are triggered in the electron and muon channels, respectively.

Collision candidates are selected by requiring a primary vertex with at least three tracks, consistent with the beam spot position. To reduce fake collision candidates from cosmic-ray or beam-halo events, the muon analysis requires the primary vertex position along the beam axis is required to be within 15 cm of the nominal position.

### 5.2 Event preparation

An analysis of a high statistics sample of minimum-bias events has shown that events can occasionally contain very localised high-energy calorimeter deposits not originating from the proton-proton collision, but e.g. from unexpected discharges in the hadronic end-cap calorimeter, and more rarely coherent noise in the electromagnetic calorimeter. Cosmic-ray muons undergoing a hard bremsstrahlung are also a potential source of localised energy deposits uncorrelated to the primary proton-proton collisions.

The occurrence of these events is very rare but can potentially impact significantly the $E_{\mathrm{T}}^{\text {miss }}$ measurement by creating high-energy tails [22]. To avoid spoiling the $E_{\mathrm{T}}^{\text {miss }}$ measurement, dedicated cleaning requirements using reconstructed jets (with the anti- $k_{t}$ algorithm [23]) in a narrow cone of size $\Delta R=0.4$ have been developed using a minimum-bias event sample. The jet properties are used as probes of the quality of the local calorimeter-energy deposit:
i) if more than $80 \%$ of the jet energy is deposited in the HEC calorimeter, $90 \%$ of the jet energy must be distributed over at least 6 calorimeter cells;
ii) if more than $95 \%$ of the jet energy is deposited in the EM calorimeter, less than $80 \%$ of the total jet energy must come from cells with an abnormal signal shape;
iii) the jet must primarily contain cells with energy deposited less than 50 ns before or after the nominal proton-proton collision time.

Events are kept only if all the jets reconstructed in the event with a transverse energy greater than 10 GeV at the EM scale fulfill the three requirements mentioned above. It was verified that these criteria remove less than one per mill of minimum-bias events and no $W \rightarrow \ell v$ events nor dijet events in Monte Carlo simulation.

For the electron channel only, the quality of the reconstruction of the energy deposited by the electron in the liquid argon calorimeter is assessed. The event is rejected if the candidate electromagnetic cluster is located in any problematic region of this detector: regions affected by major high-voltage problems, isolated cells producing a high noise signal or no signal at all, and electronic front-end boards not providing any output signal. These problems can cause extended dead regions in a given layer of the calorimeter, which may have an important impact on the energy reconstruction of the electron. To minimise the systematic uncertainty, an additional requirement is imposed such that a fiducial area around the energy clusters may not intersect that covered by a problematic front-end board if these are located in the first or second layers of the LAr EM calorimeter, where most of the electromagnetic shower energy is deposited. The loss in acceptance due to these requirements is $9 \%$ for the $W$ signal and the background.

## 6 Preselection of high transverse-energy leptons

A preselection of high transverse-energy electrons and muons is made. Electron candidates with the identification level "loose" according to the algorithm as described in Section 4.1 are required to have a cluster $E_{\mathrm{T}}>20 \mathrm{GeV}$ within the range $|\eta|<2.47$, excluding the transition region between the barrel and end-cap calorimeters ( $1.37<|\eta|<1.52$ ). Muon candidate events selected according to the algorithm described in Section 4.2 are required to have at least one combined muon with $p_{\mathrm{T}}>15 \mathrm{GeV}$ and a $p_{\mathrm{T}}$ as measured by the muon-spectrometer greater than 10 GeV , within the range $|\eta|<2.4$. The difference between the inner-detector and muon-spectrometer $p_{\mathrm{T}}$, corrected for the mean energy loss in upstream material, is required to be less than 15 GeV to increase the robustness against track reconstruction mismatches. The difference between the $z$ position of the muon track extrapolated to the beam line and the $z$ coordinate of the primary vertex is required to be less than 1 cm .

Figures 1 and 2 show the kinematic properties of these candidates and compare these to the signal and background Monte Carlo samples described in Section 3. At this stage of the selection, the candidate events are dominated by the QCD background. If these Monte Carlo distributions are normalised to the total integrated luminosity of the data, the dijet Monte Carlo cross section appears to be over-estimated by a factor of approximately 2.2 for the electron channel and a factor of 1.9 for the muon channel. This is one of the reasons why partially data-driven background estimates for the electron and muon channels are presented in Section 8. These estimates are a first attempt to measure the QCD background contribution to the $W$ channel and will greatly benefit from more statistics. The Monte Carlo distributions in Figures 1


Figure 1: Cluster $E_{T}(a)$, as well as $\eta(b)$ and $\phi(c)$ (measured in the second layer of the electromagnetic calorimeter) of electron candidates after preselection for data and Monte Carlo candidates broken down into the various signal and background components. The total number of Monte Carlo candidates is normalised to the number of observed data candidates. In Figure 1(a), the total QCD background is broken down into its constituents: hadrons misidentified as electrons, electrons from conversions, and electrons from semi-leptonic decays of heavy quarks.


Figure 2: Combined $p_{\mathrm{T}}(a), \eta(b)$, and $\phi(c)$ of muon candidates after preselection for data and Monte Carlo candidates broken down into the various signal and background components. The total number of Monte Carlo candidates is normalised to the number of observed data candidates.
and 2 have been normalised to the total number of data events, taking into account these scale factors for the QCD background. It is to be noted that all data distributions in this note are given with statistical error bars only, corresponding to $68.3 \%$ confidence intervals. These distributions show reasonable agreement in shape between data and Monte Carlo events. More details on the properties of inclusive muons are given in Ref. [24].

Figure 3 shows their transverse missing energy normalised in the same fashion as for Figures 1 and 2. Within the limited statistics afforded by the muon analysis, the $E_{\mathrm{T}}^{\text {miss }}$ distribution from the data is well reproduced by the Monte Carlo, and an excess of events around the expected signal peak region com-


Figure 3: $E_{\mathrm{T}}^{\text {miss }}$ of electron (a) and muon (b) candidates after preselection for data and Monte Carlo candidates broken down into the various signal and background components. The total number of Monte Carlo candidates is normalised to the number of observed data candidates. In Figure 3(a), the total QCD background is broken down into its constituents: hadrons misidentified as electrons, electrons from conversions, and electrons from semi-leptonic decays of heavy quarks.
pared to the background is already visible at this stage of the selection (and is the reason for the different histogramme-stacking order between the electron and the muon channel). The higher-statistics comparison of the electron analysis demonstrates that the $E_{\mathrm{T}}^{\text {miss }}$ rejection in the data for $E_{\mathrm{T}}^{\mathrm{miss}}>25 \mathrm{GeV}$ is worse than in the Monte Carlo. The source of this discrepancy is currently under investigation. It is strongly correlated to the presence of a jet faking the electron in the event and therefore not in disagreement with the conclusions of Ref. [21] which focuses on inclusive minimum-bias events.

## 7 Selection and observation of $W$ candidates

Additional requirements beyond those imposed in Section 6 are used to better discriminate potential $W \rightarrow \ell v$ events from background events. The electron identification level as described in Section 4.1 is increased to "tight" while the minimum muon combined $p_{\mathrm{T}}$ is increased to 20 GeV . Only the highest $p_{\mathrm{T}}$ lepton in the event is used.

Both the electron and muon analyses have considered the use of an isolation parameter to enhance the expected signal. However, the isolation requirements for the different channels should be considered separately, given that an electron is quite a complex object which can undergo bremsstrahlung while a muon is in some sense a simpler object primarily defined by its track. In addition, the EM calorimeter requirements for the electrons use variables which already provide some effective isolation.

A calorimeter-based isolation parameter for the electron channel defined as the total calorimeter energy within a cone of $\Delta R<0.3$ surrounding the candidate electron cluster which is then divided by the cluster $E_{\mathrm{T}}$ and a track-based isolation for the muon channel defined as the sum of inner-detector transverse momenta within a cone $\Delta R<0.4\left(\sum p_{T}^{I D}\right)$ which is then divided by the total combined muon


Figure 4: $E_{\mathrm{T}}^{\mathrm{miss}}$ versus calorimeter-isolation parameter for electron candidates (a) and track-isolation parameter for muon candidates (b) after preselection plus the "tight" requirement for electrons and muon combined $p_{\mathrm{T}}>20 \mathrm{GeV}$.
$p_{\mathrm{T}}$ are shown in Figure 4 and are plotted against the $E_{\mathrm{T}}^{\text {miss }}$ of the event. The isolation variable will be used in the electron analysis to make a data-driven estimate of the background contributions to the $W \rightarrow e v$ candidates; therefore, no form of isolation is explicitly applied in the electron-channel selection. An isolation requirement of $\sum p_{T}^{I D} / p_{T}<0.2$ is used in the muon analysis given that, after all other selections are made to identify $W$ candidates, this requirement rejects over $87 \%$ of the expected QCD background while keeping $99 \%$ of signal events. All further results shown in this section have passed the preselection requirements of Section 6, the "tight" requirement for electrons, the muon combined $p_{\mathrm{T}}>20 \mathrm{GeV}$, and this muon isolation requirement.

Additional kinematic requirements are explored in the last step of the signal selection: the $E_{\mathrm{T}}^{\text {miss }}$ of the event and the transverse mass $m_{\mathrm{T}}$ of the lepton $-E_{\mathrm{T}}^{\text {miss }}$ system defined as

$$
\begin{equation*}
m_{\mathrm{T}}=\sqrt{2 p_{\mathrm{T}}^{\ell} p_{\mathrm{T}}^{v}\left(1-\cos \left(\phi^{\ell}-\phi^{v}\right)\right)} \tag{5}
\end{equation*}
$$

where the measured $E_{\mathrm{T}}^{\text {miss }}$ components in $(x, y)$ provide the neutrino information. All Monte Carlo one-dimensional distributions shown in this section have been normalised to integrated luminosities of $6.7 \mathrm{nb}^{-1}$ and $6.4 \mathrm{nb}^{-1}$, in the electron and muon channels, respectively, using the cross sections as given in Table 1. In addition, the QCD background contributions have been scaled by factors of $1 / 2.2$ and $1 / 1.9$ in the electron and muon channels, respectively, to account for the over-estimation of the the dijet Monte Carlo cross section described in Section 6.

Figure 5 shows the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution of all electron and muon candidates passing the requirements listed above. Both distributions indicate that applying a requirement of $E_{\mathrm{T}}^{\mathrm{miss}}>25 \mathrm{GeV}$ would greatly enhance the $W$ signal over the expected background. This observation is also evident from the twodimensional plot of $E_{\mathrm{T}}^{\mathrm{miss}}$ versus electron cluster $E_{\mathrm{T}}$ and muon combined $p_{\mathrm{T}}$ shown in Figure 6. True $W \rightarrow \ell v$ events in the Monte Carlo are predominantly at high $E_{\mathrm{T}}^{\text {miss }}$ due to the escaping neutrino in the event. Although some of the QCD background may also have neutrinos in their final state, these events


Figure 5: $E_{\mathrm{T}}^{\mathrm{miss}}$ of selected electron (a) and muon (b) candidates.


Figure 6: $E_{\mathrm{T}}^{\text {miss }}$ versus the electron cluster $E_{\mathrm{T}}(a)$ and the muon combined $p_{\mathrm{T}}(b)$. For the purpose of this figure, the requirement of the muon combined $p_{\mathrm{T}}$ is lowered to 15 GeV .
mostly populate the regions of small $E_{\mathrm{T}}^{\mathrm{miss}}$.
The transverse mass of the lepton $-E_{\mathrm{T}}^{\mathrm{miss}}$ system is highly correlated to the $E_{\mathrm{T}}^{\mathrm{miss}}$ of the event as is demonstrated in Figure 7 which shows a two-dimensional plot of the $E_{\mathrm{T}}^{\mathrm{miss}}-m_{\mathrm{T}}$ plane. Figures 8 and 9 show projections of Figure 7 where the $m_{\mathrm{T}}$ of the event is shown without and with a requirement of


Figure 7: $E_{\mathrm{T}}^{\text {miss }}$ versus $m_{\mathrm{T}}$ of the lepton- $E_{\mathrm{T}}^{\text {miss }}$ system for electrons (a) and muons (b).

| Requirement | Number of <br> candidates |
| :--- | :---: |
| Triggered (Section 5) | $1.2 \times 10^{7}$ |
| Preselection (Section 6) | $2.2 \times 10^{3}$ |
| Tight electron (Section 4.1) | 77 |
| $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ | 17 |
| $m_{\mathrm{T}}>40 \mathrm{GeV}$ | 17 |

Table 2: Number of $W \rightarrow e v$ candidates remaining after each major requirement is applied.

| Requirement | Number of <br> candidates |
| :--- | :---: |
| Triggered (Section 5) | $2.8 \times 10^{5}$ |
| Preselection (Section 6) | 534 |
| $p_{\mathrm{T}}>20 \mathrm{GeV}$ | 166 |
| $\sum p_{T}^{I D} / p_{T}<0.2$ | 76 |
| $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ | 42 |
| $m_{\mathrm{T}}>40 \mathrm{GeV}$ | 40 |

Table 3: Number of $W \rightarrow \mu \nu$ candidates remaining after each major requirement is applied.
$E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$.
Tables 2 and 3 summarise the number of $W \rightarrow \ell v$ candidates remaining after each major requirement in the respective analyses described in this note. A total of 17 candidates ( $11 e^{+}$and $6 e^{-}$) pass all requirements in the electron channel and 40 candidates ( $25 \mu^{+}$and $15 \mu^{-}$) in the muon channel in the $m_{\mathrm{T}}$ region above 40 GeV . It is to be noted that the pseudorapidity dependence of the acceptance of $W^{+}$


Figure 8: $m_{\mathrm{T}}$ of the electron- $E_{\mathrm{T}}^{\text {miss }}$ system without (a) and with (b) a requirement of $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$. In Figure $8(a)$, the total QCD background is broken down into its constituents: hadrons misidentified as electrons, electrons from conversions, and electrons from semi-leptonic decays of heavy quarks.


Figure 9: $m_{\mathrm{T}}$ of the muon- $E_{\mathrm{T}}^{\text {miss }}$ system without (a) and with (b) a requirement of $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$.
and $W^{-}$production is not same and so the relative amount of positively-charged to negatively-charged $W$ bosons does not translate trivially into a cross-section ratio. Additional studies are still required (and are currently underway) before these observations can be converted into a cross section measurement.


Figure 10: Electron cluster $E_{T}(a)$ and muon combined $p_{T}(b)$ of the $W$ candidates after final selection. $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ and $m_{\mathrm{T}}>40 \mathrm{GeV}$ are required in both channels.


Figure 11: $p_{\mathrm{T}}$ of the $W$ candidates in the electron-channel (a) and muon-channel (b) after final selection. $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ and $m_{\mathrm{T}}>40 \mathrm{GeV}$ are required in both channels.

The properties of the final $W \rightarrow \ell v$ candidates are presented here. For the final selection, leptonic channels use the preselection requirements of Section 6, the "tight" requirement for electrons, the muon combined $p_{\mathrm{T}}>20 \mathrm{GeV}$ and muon isolation requirements, $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ and $m_{\mathrm{T}}>40 \mathrm{GeV}$. Figure 10
shows the electron cluster $E_{T}$ and muon combined $p_{\mathrm{T}}$ of the lepton candidates while Figure 11 shows the $p_{\mathrm{T}}$ spectrum of the $W \rightarrow \ell v$ candidates. Both channels demonstrate a clear $W$ signal over an almost negligible background. No attempt is made in this analysis to specifically identify and remove $Z$ bosons from the $W$ channel.

A few outlier events, with respect to the expected signal region, are observed in the muon channel and correspond to the events with large $W$ boson transverse momentum in Figure 11. These candidates have been inspected in detail and are consistent with the presence of a $W$ boson with a well isolated muon. Different missing energy calibrations and muon-momentum measurements have been attempted and no evident pathologies have been found.

## 8 Signal and background expectations for the $W \rightarrow \ell v$ candidates

The Monte Carlo samples discussed in Section 3 are used to provide an expectation for signal events and, in some cases for the background events. These results are summarised in Table 4. A total of 20.7 events are predicted to come from the $W \rightarrow e v$ process and 25.9 events from the $W \rightarrow \mu \nu$ process, with negligible statistical uncertainties. The difference between these two expectations stems primarily from the lower reconstruction efficiency of "tight" electrons compared to that of combined muons.

For the electron channel, the contribution from the $W \rightarrow \tau \nu$ process is expected to be small ( 0.4 events). Instead, a predominantly QCD background is expected (based on the dijet Monte Carlo, the expectation is evenly divided between heavy-quark decays, conversions, and hadrons faking electrons). $Z$ bosons decaying to electrons are expected to contribute at the $10 \%$ level of the QCD background. A partially data-driven estimate of the QCD background to the observed $W$ candidate events is made. The calorimeter isolation in a cone of $\Delta R=0.3$ divided by the electron $E_{\mathrm{T}}$ (as described in Section 7) is used as a discriminating variable in a binned maximum likelihood fit which uses Poisson statistics as described in Ref. [25]. This technique uses the prediction for the shape of the signal and the QCD background for this variable in the form of histogram templates taken from Monte Carlo samples. The distribution of this variable after the preselection is shown in Figure 12(a).

Due to the limited statistics and the very few background events, the fit cannot be performed after the final selection. Therefore only the "medium" instead of the "tight" electron identification requirement as described in Section 4.1 is applied, while the requirements on $E_{\mathrm{T}}^{\mathrm{miss}}$ and $m_{\mathrm{T}}$ are kept. Also for this reason, the signal and background templates are obtained from PYTHIA Monte Carlo samples. The fit result is shown in Fig. 12(b) and provides a background estimate of $N_{\mathrm{QCD}}$, medium $=9.8 \pm 5.7$ events, where the uncertainty contains the statistical uncertainty of the data and of the templates. The number of QCD background events after the final selection is estimated by scaling this number with the jet rejection factor for the "tight" requirement, with respect to the "medium" requirement extracted from the data for $E_{\mathrm{T}}^{\text {miss }}<20 \mathrm{GeV}$. This number is found to be $4.9 \pm 1.0$, thus giving a total QCD background of $N_{\mathrm{QCD}}$, tight $=2.0 \pm 1.2($ stat $)$. The total background in the $W$ channel is estimated to be this QCD contribution plus that coming from the $W \rightarrow \tau v$ process ( 0.4 events).

Different sources of systematic uncertainties were investigated. The QCD PYTHIA template was replaced by one obtained from the HERWIG [26] Monte Carlo. In addition, instead of dropping the "tight" requirement, the fit was performed on a sample where the "tight" requirement was applied but the $E_{\mathrm{T}}^{\mathrm{miss}}$ and $m_{\mathrm{T}}$ requirements were dropped. Finally, the number of bins used in the fit was varied in a large range. The observed variations are all small compared to the uncertainty of the fit which is to a large extent statistical. Therefore, the number of QCD background events as estimated by this template method is $N_{\mathrm{QCD}}=2.0 \pm 1.2(\mathrm{stat}) \pm 0.4$ (syst). The predicted number of QCD background events based on the dijet Monte Carlo given in Table 1 scaled by the factor of $1 / 2.2$ (as described in Section 6) is 0.8 events and so is in good agreement with this measurement.

An alternative estimate of the QCD background has been derived with the following data-driven


Figure 12: (a) Calorimeter isolation/ $E_{\mathrm{T}}$ (as described in Section 7) after preselection. The total number of Monte Carlo candidates is normalised to the number of observed data candidates. (b) Result of the template fit where the event selection contains all requirements but that of the "tight" electron (these are "medium" electrons). The Monte Carlo distributions are scaled to the result of the fit.
method. The ratio between the number of electrons passing the "tight" selection and the number of electrons passing the "loose" but failing the "medium" selection (as described in Section 4.1) is measured in data for events with $E_{\mathrm{T}}^{\mathrm{miss}}<10 \mathrm{GeV}$. The estimated number of QCD events after the signal selection is then obtained as the number of observed events with one "loose" electron failing "medium" requirements, which pass the signal selection requirements on $E_{\mathrm{T}}^{\text {miss }}$ and transverse mass. Several sources of systematic uncertainties have been considered such as the limited statistics of the Monte Carlo samples, the expected contamination of $W$ and $Z$ events in the control regions, and the stability of the accuracy of the estimate varying each individual component (hadron, conversion, and heavy flavour) in the Monte Carlo sample by a factor of two. The size of QCD background in the signal candidates selection is estimated to be $1.2 \pm 0.5$ events and is in agreement with the result of the template method quoted above.

For the muon channel, the total background estimate is 2.8 events, primarily coming from multijets and $Z \rightarrow \mu \mu$ decays ( $36 \%$ each of all the background). Other sources of backgrounds are $24 \%$ from $W \rightarrow \tau v$ decays, $3 \%$ from top production and $1 \%$ from $Z \rightarrow \tau \tau$ decays. Given the high uncertainty in the Monte Carlo dijet cross section, this source of background has been also measured in data using the distribution of missing energy versus isolation prior to the transverse mass requirement, as described below. The isolation distribution for preselected events is shown in Figure 13.

The primary assumption of this method to extract the multijet component of the total background is that the $E_{\mathrm{T}}^{\text {miss }}$ and the lepton isolation are uncorrelated. The $E_{\mathrm{T}}^{\text {miss }}$ versus track-isolation plane is divided into four separate regions defined by the same $E_{\mathrm{T}}^{\mathrm{miss}}$ and isolation requirements as for the $W$ selection (Figure 4(b)). The background contribution to the $W$ signal region is obtained from a similarity relationship between the contents in the four regions of the $E_{\mathrm{T}}^{\text {miss }}$-isolation space. The calculation is corrected for the contributions from the signal and the electroweak backgrounds described above.

This method yields a jet background estimate of $1.3 \pm 1.2$ events if no $m_{\mathrm{T}}$ requirement is imposed or $1.0 \pm 0.5$ (stat) $\pm 0.7$ (syst) events if $m_{\mathrm{T}}>40 \mathrm{GeV}$. The systematic uncertainty in this method is due to


Figure 13: Track-isolation variable $\sum p_{T}^{I D} / p_{T}(a)$ and $E_{T}^{\text {miss }}$ distribution of non-isolated events (b) after muon preselection. The total number of Monte Carlo candidates is normalised to the number of observed data candidates.
the correlation between the two variables used and has been estimated from the difference between the number of predicted and observed events in the signal region in a consistency check with Monte Carlo QCD sample. Since this technique is also sensitive to poorly reconstructed events faking muons as well as pion and kaon decays, this estimation is used for the final number of expected events.

An alternative estimation of the multijet background has been made by measuring the QCD background normalisation in data. The control sample used is obtained by reversing the isolation requirement after preselection. The assumption is that these events are dominated by muons from QCD background events. The background normalisation is taken from the comparison of the distributions of $E_{\mathrm{T}}^{\mathrm{miss}}$, in both data and jet background Monte Carlo samples. These are shown in Figure 13(b), where the QCD distribution has been normalised to the numbers of event in the control sample. The data and Monte Carlo shapes appear to agree well and an overall scale factor of Monte Carlo QCD cross section to data of 0.54 is measured. This method derives a background estimate of $0.2 \pm 0.1$. A value in agreement with this estimate is found when increasing the muon transverse momentum requirement to 20 GeV . An independent study using dijet Monte Carlo predicts that the background contamination from pion and kaon decays is $0.15 \pm 0.15$, which is well within the direct estimation from data.

All muon candidate events were inspected individually, verifying the main reconstruction parameters. Distributions of hit multiplicities in inner-detector and muon-spectrometer tracks, their track-matching $\chi^{2}$, and the difference in the transverse momentum measurement between the two sub-detectors were compared in data and Monte Carlo. A good agreement was found for all of these items. The hypothesis that a cosmic ray overlays with the collision was carefully verified by looking at the timing properties of muon tracks. TRT, tile calorimeter and MDT time measurements where analysed and no clear indication of cosmic contamination was found.

A fair degree of uncertainty still exits in these background estimates due to the statistically limited control samples and Monte Carlo simulations, and also from leading-order jet cross sections and fragmentation functions.

|  | $W \rightarrow e v$ channel | $W \rightarrow \mu \nu$ channel |
| :--- | :--- | :--- |
| Observed | 17 | 40 |
| Expected | $23.1 \pm 1.2($ stat $) \pm 1.7($ syst $) \pm 4.6($ lumi $)$ | $28.7 \pm 0.5($ stat $) \pm 3.9($ syst $) \pm 5.7(\mathrm{lumi})$ |
| Signal | $20.7 \pm 1.7($ syst $) \pm 4.1($ lumi $)$ | $25.9 \pm 3.6($ syst $) \pm 5.2($ lumi $)$ |
| Bkg | $2.4 \pm 1.2($ stat $) \pm 0.4($ syst $) \pm 0.5($ lumi $)$ | $2.8 \pm 0.5($ stat $) \pm 0.8($ syst $) \pm 0.6(\mathrm{lumi})$ |

Table 4: Numbers of observed and expected events from the $W \rightarrow \ell v$ channel. The statistical uncertainty is represented by "stat". The "syst" uncertainty is given for both the measured background and the signal prediction as described in the text. The "lumi" uncertainty refers to the contribution due to the luminosity determination.

The systematic uncertainties for the electron and muon channels on the number of expected events come from a number of sources. The dominant one is the luminosity determination for which a $20 \%$ scale uncertainty is used for both channels. Other sources of inefficiencies contributing to the total systematic error are analysis dependent. For the electron channel, data-Monte Carlo comparisons estimate the lepton identification uncertainties at $5 \%$ and the choice of $E_{\mathrm{T}}^{\mathrm{miss}}$ requirement at $5 \%$. In addition, an uncertainty of $4 \%$ is attributed to the theoretical cross section and on the acceptance from the parton distribution functions. Trigger inefficiencies are considered to be negligible in comparison. For the muon channel, several sources of uncertainties were considered and added in quadrature resulting in an overall $14 \%$ systematic uncertainty. The following contributions are included. The uncertainty on muon reconstruction efficiency is estimated to be $10 \%$. The single-muon trigger efficiency as measured in data is calculated as an average of the values measured in RPC and TGC detectors, weighted by the relative number of events in their acceptance. The ratio of trigger efficiency as measured in data and in Monte Carlo samples is 0.92 . This scale factor has been used to correct the Monte Carlo predictions in this note. A $7 \%$ uncerainty is attributed to this muon trigger scale factor. A $5 \%$ uncertainty is assigned to the muon resolution. Finally, a $4 \%$ uncertainty is assigned to the theoretical cross section and on the acceptance from the parton distribution functions.

The total number of events expected to pass all selection requirements in the $W \rightarrow e v$ channel is $23.1 \pm 1.2($ stat $) \pm 1.7($ syst $) \pm 4.6($ lumi $)$ and is $28.7 \pm 0.5($ stat $) \pm 3.9$ (syst) $\pm 5.7$ (lumi) in the $W \rightarrow \mu v$ channel. The numbers of observed and expected events in both channels are summarised in Table 4.

## 9 Observation of $Z$ candidates

A search for $Z$ candidates was also performed in both the electron and muon channels. The preselection specifications listed in Section 6 are first applied. Subsequent requirements are made to specifically search for lepton pairs consistent with being produced from the decay of a $Z$ boson. For the electron channel, leptons are required to be of opposite charge and each lepton must pass at least the "medium" requirements as presented in Section 4.1. For the muon channel, the selection is loosened compared to the $W$ search: only one of the muon candidates is required to have a minimum muon combined $p_{\mathrm{T}}$ above 20 GeV . The other muon minimum $p_{\mathrm{T}}$ threshold remains at 15 GeV and the pseudorapidity requirement of this second muon is relaxed to $|\eta|<2.5$. Muon candidates must have opposite charge and a muon isolation parameter $\sum p_{T}^{I D} / p_{T}<0.2$. Within the invariant mass window $m_{\ell \ell}=80-100 \mathrm{GeV}$, one candidate with an invariant mass of 91.4 GeV passes these requirements in the electron channel and two candidates with invariant masses of 80.2 GeV and 87.6 GeV in the muon channel. No events were found in the electron selection outside this mass window and only one event at lower mass in the muon selection.

The $Z \rightarrow \ell \ell$ Monte Carlo samples discussed in Section 3 are used to provide an expectation for signal events. For the electron channel, a total of $1.6 \pm 0.1$ (syst) $\pm 0.3$ (lumi) signal events with a negligible statistical uncertainty are expected for an integrated luminosity of $6.7 \mathrm{nb}^{-1}$. This estimate includes a $20 \%$ uncertainty on the luminosity, a $5 \%$ systematic uncertainty on the acceptance and efficiency, and a $4 \%$ contribution for the theoretical cross section uncertainty and on the acceptance from the parton distribution functions. For the muon channel, a total of $3.2 \pm 0.7$ (syst) $\pm 0.6$ (lumi) signal events with a negligible statistical uncertainty are expected for an integrated luminosity of $7.9 \mathrm{nb}^{-1}$. Apart from the $20 \%$ uncertainty in luminosity determination, the primary source of systematic uncertainty in this prediction is the reconstruction efficiency. Since the final state in $Z \rightarrow \mu \mu$-like events contains two muons, the uncertainties in their reconstruction efficiencies are added linearly, yielding an uncertainty on the event reconstruction efficiency of $20 \%$. This number assumes that the uncertainties are fully correlated between the two muons. The uncertainty in the trigger efficiency scaling factor is $4 \%$. The other sources of systematics are the same as for the $W$ channel. These contributions are added in quadrature resulting in the final number given above.

The background Monte Carlo samples in Section 3 as such have insufficient statistics to provide a direct estimate of the expected background events in the $Z \rightarrow e e$ channel within the mass window $80<$ $m_{e e}<100 \mathrm{GeV}$. A partially data-derived estimate is made. For the electron channel, the QCD background Monte Carlo sample may be used to estimate the number of pairs of leptons that both pass the "loose" electron requirement, in the appropriate mass range. A data-derived "loose" to "medium" rejection factor is then used to estimate the expected number of lepton pairs which both pass the nominal $Z \rightarrow e e$ requirements. The ratio of "medium" to "loose" electrons with $p_{\mathrm{T}}>20 \mathrm{GeV}$, reconstructed using the standard electron algorithm of Section 4.1 and within the $\eta$ acceptance of the detector is measured in data to be $0.40 \pm 0.16$. This rejection, quoted here as its reciprocal, is consistent with the rejection measured from electrons in the QCD background Monte Carlo. In the Z mass window $80<m_{e e}<100 \mathrm{GeV}$, the Monte Carlo predicts there to be $0.14 \pm 0.01$ QCD background events in the opposite-charge invariant mass distribution for "loose" lepton pairs. By applying the data-derived rejections to each electron in these pairs, a background estimate of 0.01 "medium" pairs in the opposite-charge distribution in the $Z$ mass window is derived.

The total number of expected background events within the mass window $80<m_{\mu \mu}<100 \mathrm{GeV}$ in the muon channel after all requirements as estimated from Monte Carlo samples described in Table 1 is $(2.1 \pm 0.8$ (syst) $\pm 0.4$ (lumi) $) \times 10^{-4}$, where the dominant source is top-pair production $(52 \%)$. The QCD contribution is $38 \%$ and other sources are negligible.

## 10 Summary

This note presents an observation by the ATLAS experiment of $57 \mathrm{~W} \rightarrow \ell v$ candidates produced from $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions at the LHC. These results, collected over a seven-week period from March to May 2010, correspond to a total integrated luminosity of $6.7 \mathrm{nb}^{-1}$ for the $W \rightarrow e v$ channel, and $6.4 \mathrm{nb}^{-1}$ for the $W \rightarrow \mu \nu$ channel. These results are in agreement with the expectation of 51.8 events. Three $Z \rightarrow \ell \ell$ candidates were observed with an expectation of 4.8 given the integrated luminosities of $6.7 \mathrm{nb}^{-1}$ for the $Z \rightarrow e e$ channel and $7.9 \mathrm{nb}^{-1}$ for the $Z \rightarrow \mu \mu$ channel. The number of events observed is consistent with the expectation.

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# Measurement of the $W \rightarrow \ell v$ production cross-section and observation of $Z \rightarrow \ell \ell$ production in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

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#### Abstract

This note describes the first measurement of the $W \rightarrow \ell v$ production cross section and an observation of $Z \rightarrow \ell \ell$ production, where $\ell=e, \mu$, by the ATLAS experiment. These results are based on $118 \mathrm{~W} \rightarrow \ell v$ candidates and $14 Z \rightarrow \ell \ell$ candidates, produced in $\sqrt{s}=$ 7 TeV proton-proton collisions at the LHC and correspond to a total integrated luminosity of approximately $17 \mathrm{nb}^{-1}$. The total inclusive $W$-boson production cross section times the leptonic branching ratio is measured to be ( $8.5 \pm 1.3$ (stat) $\pm 0.7$ (syst) $\pm 0.9$ (lumi)) nb for the $W \rightarrow e v$ channel and $(10.3 \pm 1.3$ (stat) $\pm 0.8$ (syst) $\pm 1.1$ (lumi)) nb for the $W \rightarrow \mu \nu$ channel. This constitutes the first $W$ cross-section measurement by ATLAS in proton-proton collisions and the result obtained is in agreement with theoretical calculations based on NNLO QCD. In addition the expected charge asymmetry between the cross sections for $W^{+}$and $W^{-}$production is experimentally confirmed.


## 1 Introduction

The experimental study of the electroweak gauge bosons has a history of about thirty years. The $W$ and the $Z$ particles were initially discovered and measured at the CERN proton-antiproton collider in 1983 [1, 2, 3, 4]. During the early 1990's, the $Z$ properties were measured in great detail at the high energy $e^{+} e^{-}$colliders LEP and SLC [5]. In the second half of that decade, an energy increase of LEP enabled the study of $W$ bosons produced in pairs. The Tevatron proton-antiproton collider has been accumulating $W$ and $Z$ events over the last twenty years [6, 7]. The results of these programmes include high-precision measurements of the $W$ and $Z$ mass, width, and couplings, as well as detailed information on their production in proton-antiproton collisions. The current uncertainties on the intrinsic properties of the $W$ boson are about ten times larger than on their $Z$ counterparts [8].

The $W$ and $Z$ bosons are expected to be produced abundantly at the Large Hadron Collider (LHC) [9], and for the first time in proton-proton collisions. This eventual large dataset and the high LHC energy will allow for detailed measurements of their production properties at a previously unexplored kinematic domain of low parton momentum fraction at a high energy scale. These conditions, together with the particular nature of the collisions, will provide new insights on the proton properties, tests of perturbative QCD calculations, and ultimately a precise determination of the mass of the $W$ boson [10, 11]. In this process, the well-known properties of the $Z$ boson will provide significant constraints in the determination of the performance of the collider experiments at the LHC; its known mass, width and leptonic decays can be exploited to measure precisely the detector energy and momentum scale, resolution, as well as lepton identification and trigger efficiencies.

This note details an observation by the ATLAS [12] experiment of $46 \mathrm{~W} \rightarrow e v$ and $72 \mathrm{~W} \rightarrow \mu \nu$ candidates produced from the $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions of the LHC, resulting from a total integrated luminosity of approximately $17 \mathrm{nb}^{-1}$. A total of five $Z \rightarrow e e$ and nine $Z \rightarrow \mu \mu$ candidates were also observed. These data were collected over a ten-week period from March to June 2010. The uncertainty on the luminosity determination is estimated to be $11 \%$ [13]. The results presented in this note supersede those of Ref. [14].

## 2 The ATLAS detector

The ATLAS detector [12] at the LHC comprises a thin superconducting solenoid surrounding the innerdetector cavity and three large superconducting toroids arranged with an eight-fold azimuthal coil symmetry placed around the calorimeters, forming the basis of the muon spectrometer.

In this note, the nominal interaction point is defined as the origin of the coordinate system, while the anti-clockwise beam direction defines the $z$-axis and the $x-y$ plane is transverse to the beam direction. The positive $x$-axis is defined as pointing from the interaction point to the centre of the LHC ring and the positive $y$-axis is defined as pointing upwards. The azimuthal angle $\phi$ is measured around the beam axis and the polar angle $\theta$ is the angle from the beam axis. The pseudorapidity is defined as $\eta=-\ln \tan (\theta / 2)$. The transverse momentum $p_{\mathrm{T}}$, the transverse energy $E_{\mathrm{T}}$, and the transverse missing energy $E_{\mathrm{T}}^{\mathrm{miss}}$ are defined in the $x-y$ plane. The distance $\Delta R$ in the $\eta-\phi$ space is defined as $\Delta R=\sqrt{\Delta \eta^{2}+\Delta \phi^{2}}$.

The Inner-Detector (ID) system is immersed in a 2 T axial field and provides tracking information on charged particles in a pseudorapidity range matched by the precision measurements of the electromagnetic calorimeter. The silicon tracking detectors, pixel and silicon microstrip (SCT), cover the pseudorapidity range $|\eta|<2.5$. The highest granularity is achieved around the vertex region using the pixel detectors. Typically three pixel layers are crossed by each track. For the SCT, eight strip layers (providing four space points) are crossed by each track in the barrel region. A large number of hits (typically 36 per track) is provided by the Transition Radiation Tracker (TRT), which enables track-following up to $|\eta|=2.0$. The electron identification information is provided by the detection of transition radiation in
the xenon-based gas mixture of the TRT straw tubes.
The calorimeter system covers the pseudorapidity range $|\eta|<4.9$, using a variety of detector technologies. The lead/liquid-argon (LAr) electromagnetic (EM) calorimeter is divided into a barrel part $(|\eta|<1.475)$ and two end-cap components $(1.375<|\eta|<3.2)$. The pseudorapidity range $1.37<|\eta|<$ 1.52 is considered as the transition region between the barrel and end-cap and is omitted in this analyses. Over the region devoted to precision physics ( $|\eta|<2.5$ ), the EM calorimeter is segmented in three sections in depth. The remaining portion of the EM calorimeter, known as the end-cap inner wheel, is segmented in two sections in depth and has a coarser lateral granularity than for the rest of the acceptance. In the region of $|\eta|<1.8$, a thin LAr presampler detector is used to correct for the energy lost by electrons, positrons, and photons upstream of the calorimeter. The hadronic tile calorimeter is placed directly outside the EM calorimeter envelope. This steel/scintillating-tile detector consists of a barrel covering the region $|\eta|<1.0$, and two extended barrels in the range $0.8<|\eta|<1.7$. The copper-LAr Hadronic End-cap Calorimeter (HEC) consists of two independent wheels per end-cap ( $1.5<|\eta|<3.2$ ), located directly behind the end-cap electromagnetic calorimeter. The Forward Calorimeter (FCal) consists of three modules in each end-cap: the first, made of copper-LAr, is optimised for electromagnetic measurements, while the other two, made of tungsten-LAr, measure primarily the energy of hadronic interactions.

The muon spectrometer is based on the magnetic deflection of muon tracks in the large superconducting air-core toroid magnets, instrumented with separate trigger and high-precision tracking chambers. A system of three large air-core toroids, a barrel and two end-caps, generates the magnetic field for the muon spectrometer in the pseudorapidity range of $|\eta|<2.7$. In the barrel region, tracks are measured in chambers arranged in three cylindrical layers around the beam axis; in the transition and end-cap regions, the chambers are installed in planes perpendicular to the beam, also in three layers. Over most of the $\eta$-range, a precision measurement of the track coordinates in the principal bending direction of the magnetic field is provided by Monitored Drift Tubes (MDT's). At large pseudorapidities, Cathode Strip Chambers (CSC's) with higher granularity are used in the innermost plane over $2.0<|\eta|<2.7$, to withstand the demanding rate and background conditions expected with the LHC operation at the nominal luminosity and centre-of-mass energy. The muon trigger system, which covers the pseudorapidity range $|\eta|<2.4$, consists of Resistive Plate Chambers (RPC's) in the barrel $(|\eta|<1.05)$ and Thin Gap Chambers (TGC's) in the end-cap regions ( $1.05<|\eta|<2.4$ ), with a small overlap in the $|\eta|=1.05$ region.

The first-level (L1) trigger system uses a subset of the total detector information to make a decision on whether or not to process an event. Details about the L1 calorimeter and muon trigger systems used in the analysis of the $W$ and $Z$ candidates are provided in Section 5.

## $3 W, Z$ processes and sources of background

The results presented in this note are compared to expectations based on Monte Carlo simulations. The signal and background samples used in this note were generated at $\sqrt{s}=7 \mathrm{TeV}$ with PYTHIA [15] using MRSTLO* [16] parton distribution functions (PDF), then simulated with GEANT4 [17] and fully reconstructed. Details of these samples are summarised in Table 1.

The $W$ and $Z$ production cross sections times their respective $W \rightarrow \ell \nu$ and $Z / \gamma^{*} \rightarrow \ell \ell$ decay branching ratios used in this study are calculated to next-to-next-to-leading order (NNLO) in QCD using the FEWZ program [18] with the MSTW2008 set of parton distribution functions [19]. The dilepton invariant mass of the $Z / \gamma^{*} \rightarrow \ell \ell$ process is required to be greater than 60 GeV . In contrast to proton-antiproton collisions, the cross sections for $W^{+}$and $W^{-}$production measured with proton-proton collisions are asymmetric due to the absence of valence anti-quarks in the proton. These values are:

$$
\begin{equation*}
\sigma_{W \rightarrow \ell v}^{N N L O}=10.46 \mathrm{nb} \quad\left(\sigma_{W^{+} \rightarrow \ell^{+} v}^{N N L O}=6.16 \mathrm{nb} \text { and } \sigma_{W^{-} \rightarrow \ell^{-} v}^{N N L O}=4.30 \mathrm{nb}\right) \text { and } \sigma_{Z / \gamma^{*} \rightarrow \ell \ell}^{N N L O}=0.99 \mathrm{nb} \tag{1}
\end{equation*}
$$

An overall uncertainty of the NNLO $Z$ and $W$ cross sections of $4 \%$ has been estimated using the MSTW2008NNLO PDF error eigenvectors at the $90 \%$ C.L. limit, the NNLO HERAPDF1.0 $\alpha_{s}$ variations [20], and normalisation and scale variations. The obtained uncertainty covers the NNLO crosssection predictions using the ABKM09 fits [21].

The background contributions expected from jet production via QCD processes (referred to as "QCD background" in this note) have significant components from semi-leptonic decays of heavy quarks, hadrons misidentified as leptons, and in the case of the electron channel, electrons from conversions. For both the electron and muon channels, these sources of background have been obtained from dijet samples.

In the case of the $W$ analysis, $W$ events decaying into $\tau$-leptons with subsequent leptonic $\tau$ decays are also expected to contribute in both channels. Contributions from $Z \rightarrow \mu \mu$ decays are significant in the muon channel but less so for the corresponding $Z \rightarrow e e$ decays in the electron channel. The large $\eta$ coverage of the calorimeter system is less likely to generate $E_{\mathrm{T}}^{\text {miss }}$ in the electron channel than $Z \rightarrow \mu \mu$ decays in the muon channel. The muon channel additionally takes into account contributions from $Z \rightarrow$ $\tau \tau$ decays and from $t \bar{t}$ events involving at least one semi-leptonic decay, though these contributions are small. The $t \bar{t}$ contribution in the electron channel is estimated to be $0.4 \%$ of the total electroweak signal. The cosmic ray contribution to the overall background in the muon channel is estimated to be very small ( $0.10 \pm 0.04$ ) and is neglected in this analysis.

## 4 Object reconstruction

### 4.1 Electrons

### 4.1.1 Standard electrons

The ATLAS standard electron/photon reconstruction and identification algorithm [22] is designed to provide various levels of background rejection optimised for high identification efficiencies for calorimeter transverse energy $E_{\mathrm{T}}>20 \mathrm{GeV}$, over the full acceptance of the inner-detector system. Electron reconstruction begins with a seed cluster of energy of $E_{\mathrm{T}}>2.5 \mathrm{GeV}$ in the second layer of the electromagnetic calorimeter. This cluster of size $\Delta \eta \times \Delta \phi=0.075 \times 0.125$ is selected by a sliding window algorithm. A matching track, extrapolated to the middle EM calorimeter layer, is searched for in a broad window of $\Delta \eta \times \Delta \phi=0.05 \times 0.1$ amongst all reconstructed tracks with $p_{\mathrm{T}}>0.5 \mathrm{GeV}$. The closest-matched track to this layer's cluster barycentre is kept as that belonging to the electron candidate. The final electron candidates have cluster sizes of $\Delta \eta \times \Delta \phi=0.075 \times 0.175$ in the barrel calorimeter and $0.125 \times 0.125$ in the end-cap. The total transverse energy of these clusters is the $E_{\mathrm{T}}$ used in this analysis.

The baseline electron identification selections [22] are based on criteria using calorimeter and tracker information and have been optimised in 10 bins in $\eta$ and 11 bins in $E_{\mathrm{T}}$. Three reference sets of requirements ("loose", "medium", and "tight") have been chosen, providing progressively stronger jet rejection at the expense of some identification efficiency loss. Each set adds additional constraints to the previous requirements:

- "Loose": this basic selection uses EM shower shape information from the second layer of the EM calorimeter (lateral shower containment and shower width) and energy leakage into the hadronic calorimeters as discriminant variables. This set of requirements provides high and uniform identification efficiency but a low background rejection;

| Physics process | Cross section (nb) [ $\times$ BR] | Luminosity ( $\mathrm{nb}^{-1}$ ) |
| :---: | :---: | :---: |
| $\mathrm{W} \rightarrow e v$ | 10.46 | $6.7 \times 10^{5}$ |
| $\mathrm{W} \rightarrow \mu \nu$ | 10.46 | $6.7 \times 10^{5}$ |
| $\mathrm{W} \rightarrow \tau \nu$ (electron channel analysis) | 10.46 | $1.9 \times 10^{5}$ |
| $\mathrm{W} \rightarrow \tau \nu \rightarrow \mu \nu \nu$ | 3.68 | $3.1 \times 10^{5}$ |
| $\mathrm{Z} \rightarrow e e\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.99 | $4.8 \times 10^{6}$ |
| $\mathrm{Z} \rightarrow \mu \mu\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.99 | $5.1 \times 10^{6}$ |
| $\mathrm{Z} \rightarrow \tau \tau\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.99 | $2.0 \times 10^{6}$ |
| $t \bar{t}$ | 0.16 | $2.5 \times 10^{6}$ |
| Dijet (electron channel, $\hat{p}_{\mathrm{T}}>15 \mathrm{GeV}$ ) | $1.15 \times 10^{6}$ | 100 |
| Dijet (muon channel, $8<\hat{p}_{\mathrm{T}}<17 \mathrm{GeV}$ ) | $9.86 \times 10^{6}$ | 0.05 |
| Dijet (muon channel, $17<\hat{p}_{\mathrm{T}}<35 \mathrm{GeV}$ ) | $6.78 \times 10^{5}$ | 0.74 |
| Dijet (muon channel, $35<\hat{p}_{\text {T }}<70 \mathrm{GeV}$ ) | $4.10 \times 10^{4}$ | 12.20 |
| Dijet (muon channel, $70<\hat{p}_{\mathrm{T}}<140 \mathrm{GeV}$ ) | $2.20 \times 10^{3}$ | 227.74 |
| Dijet (muon channel, $140<\hat{p}_{\text {T }}<280 \mathrm{GeV}$ ) | $0.88 \times 10^{2}$ | $5.70 \times 10^{3}$ |
| Dijet (muon channel, $280<\hat{p}_{\mathrm{T}}<1120 \mathrm{GeV}$ ) | 2.35 | $2.13 \times 10^{5}$ |
| $b \bar{b}$ (muon channel, $\hat{p}_{T}>15 \mathrm{GeV}$ ) | $7.39 \times 10^{4}$ | $59 \times 10^{3}$ |
| $c \bar{c}$ (muon channel, $\hat{p}_{\mathrm{T}}>15 \mathrm{GeV}$ ) | $2.84 \times 10^{4}$ | $53 \times 10^{3}$ |

Table 1: Signal and background Monte Carlo samples used in the electron and muon channel analyses, including the production cross section (multiplied by the relevant branching ratios (BR)) and the integrated luminosity of the samples. The variable $\hat{p}_{T}$ is the transverse momentum of the partons involved in the hard scatter. $W$ and $Z$ cross sections are given at NNLO, the $t \bar{t}$ cross section is given at next-toleading order (plus next-to-next-to-leading log), and the dijet and heavy quark cross sections are given at leading order (LO).

- "Medium": this selection provides additional hadronic rejection by evaluating the energy deposit patterns in the first layer of the EM calorimeter (the shower width and the ratio of the energy difference associated with the largest and second largest energy deposit over the sum of these energies), track quality variables (number of hits in the pixel and silicon trackers, the transverse impact parameter) and a cluster-track matching variable ( $\Delta \eta$ between the cluster and the track extrapolated to the first layer of the EM calorimeter);
- "Tight": this selection further rejects charged hadrons and secondary electrons from conversions by fully exploiting the electron identification potential of the ATLAS detector. It makes requirements on the ratio of cluster energy to track momentum, on the number of hits in the TRT, and on the ratio of high-threshold to the total number of hits in the TRT. Electrons from conversions are rejected by requiring at least one hit in the first layer of the pixel detector. A conversion-flagging algorithm is also used to further reduce this contribution. The impact-parameter requirement applied in the medium selection is further tightened at this level.

Using $Z \rightarrow e e$ signal and QCD dijet Monte Carlo samples for electrons with $E_{T}>20 \mathrm{GeV}$ within the range $|\eta|<2.47$ and excluding the transition region between the barrel and end-cap calorimeters ( $1.37<|\eta|<1.52$ ), the expected identification efficiencies are estimated to be $94 \%, 90 \%$, and $72 \%$ with rejection factors against background jets with true $E_{\mathrm{T}}>20 \mathrm{GeV}$ of 1100,6800 , and 92000 for "loose", "medium", and "tight" electron identification, respectively [22].

### 4.1.2 Forward electrons

In contrast to the standard electron selection discussed above, forward electrons are reconstructed outside the range of the ATLAS inner-detector system where no tracking is available and so an alternative topological clustering algorithm (discussed in Section 4.3) is used. The electron candidates with $|\eta|>2.5$ are reconstructed if a cluster with $E_{\mathrm{T}}>5 \mathrm{GeV}$ is present in the calorimeter. The direction of the electron candidate cluster is defined by the barycenter of the cells belonging to the calorimeter cluster. The total energy deposited in the calorimeter is taken to be the energy of the electron candidate. Two classes of forward electrons are defined: "loose-forward" electrons with longitudinal and transverse shower profile consistent with an electron shower and "tight-forward" electrons that have further requirements based on shower shape variables. This "tight-forward" electron identification uses six discriminating variables defined using cluster moments or a combination of them as discussed in Ref [22].

### 4.2 Muons

The ATLAS muon identification and reconstruction algorithms take advantage of the multiple subdetector technologies which provide complementary approaches and cover pseudorapidities up to 2.7 over a wide $p_{\mathrm{T}}$ range [10].

The stand-alone muon reconstruction is based entirely on muon-spectrometer information, independently of whether or not this muon-spectrometer track is also reconstructed in the inner detector. The muon reconstruction is initiated locally in a muon chamber by a search for straight line track segments in the bending plane. Hits in the precision chambers are used and the segment candidates are requested to point to the centre of ATLAS. The hit coordinate $\phi$ in the non-bending plane measured by the trigger detectors is associated to the segment when available. A minimum of two track segments in different muon stations are combined to form a muon track candidate using three-dimensional tracking in the magnetic field. The track parameters $\left(p_{\mathrm{T}}, \eta, \phi\right.$, distance of closest approach to the primary vertex along the beam axis and transverse to it) are obtained from the muon spectrometer track fit and are extrapolated to the interaction point taking into account both multiple scattering and energy loss in the calorimeters. For the latter, the reconstruction utilises either a parameterisation or actual measurements of calorimeter energy losses, together with a parameterisation of energy loss in the inert material. The typical muon energy loss in the calorimeters is 3 GeV . The stand-alone muon reconstruction algorithms use the least-squares formalism to fit tracks in the muon spectrometer and most material effects are directly integrated into the $\chi^{2}$ function.

The combined muon reconstruction associates a stand-alone muon spectrometer track to an innerdetector track, that measures the bending of the muon within the solenoid, using the pixel, SCT and TRT detectors. The association between the stand-alone and inner-detector tracks is performed using a $\chi^{2}$-test, defined from the difference between the respective track parameters weighted by their combined covariance matrices. The parameters are evaluated at the point of closest approach to the beam axis. The combined track parameters are derived either from a statistical combination of the two tracks or from a refit of the full track. To validate the results presented in this note, these two independent reconstruction chains were exercised, leading to a good agreement. The results presented here are based on the one which relies on the statistical combination of muon-spectrometer and inner-detector measurements.

Detailed studies of the muon performance in collision data have been done. They are limited to the momentum region below about 20 GeV due to the small size of the data samples available in the higher $p_{\mathrm{T}}$ domain. The studies are based on relative measurements of the muon track properties taking the inner detector as a reference. In the region of $p_{\mathrm{T}}$ between 10 GeV and 20 GeV , the relative momentum scale difference is found to be below $2 \%$ in both barrel and endcap regions, while the relative momentum resolution is measured to be $5 \%$ in the barrel and $8.5 \%$ in the endcap regions [23]. This value in the end-cap region may be explained by alignment issues. In the barrel region, chambers have been better
aligned with cosmic rays [24]; however, additional inert material is possibly needed to account for the observed sagitta and resolution dependence on momentum. Different complementary approaches have been inspected to measure the relative muon reconstruction efficiency in data. Results are in agreement with Monte Carlo expected values within 2-3\%. The results based on these analyses have been used in the systematic uncertainty evaluation reported in Section 10.2.2. Studies with collision data are underway but are currently limited by the number of high- $p_{\mathrm{T}}$ muons collected so far [23].

### 4.3 Transverse missing energy

The transverse missing energy ( $E_{\mathrm{T}}^{\text {miss }}$ ) reconstruction used in the electron channel is based on calorimeter information. This relies on a cell-based algorithm which sums the electromagnetic-scale energy deposits of calorimeter cells inside three-dimensional topological clusters [25]. The EM scale is the energy deposited in the calorimeter calculated under the assumption that all processes are purely electromagnetic in nature. These clusters are then corrected to take into account the different response to hadrons than to electrons or photons, dead material losses and out of cluster energy losses [26]. These topological clusters are built around energy $E>4 \sigma_{\text {noise }}$ seeds, where $\sigma_{\text {noise }}$ is the Gaussian width of the cell energy distribution in randomly triggered events, by iteratively gathering neighbouring cells with $E>2 \sigma_{\text {noise }}$ and, in a final step, by adding all direct neighbours of these accumulated secondary cells. The $x$ - and $y$-components of the calorimeter $E_{\mathrm{T}}^{\mathrm{miss}}$ term are calculated by summing over the transverse energies measured in these topological cluster cells $i$ :

$$
\begin{equation*}
E_{x, y}^{\text {Electron,miss }}=E_{x, y}^{\text {Calo,miss }}=-\sum_{i} E_{x, y} \tag{2}
\end{equation*}
$$

The $E_{\mathrm{T}}^{\text {miss }}$ used in the muon channel is calculated from the reconstructed momenta of muons measured in the range of pseudorapidity $|\eta|<2.7$ and the calorimeter term as given in Eq. 2:

$$
\begin{equation*}
E_{x, y}^{\text {Muon,miss }}=-\left(\sum_{\text {Muons }} E_{x, y}+\sum_{i} E_{x, y}\right)=-\left(\sum_{\text {isolated }} p_{x, y}+\sum_{n o n-i s o l a t e d} p_{x, y}\right)+E_{x, y}^{\text {Calo,miss }}, \tag{3}
\end{equation*}
$$

where non-isolated muons are those within a distance $\Delta R \leq 0.3$ of a jet in the event. The $p_{\mathrm{T}}$ of an isolated muon is determined from the combined measurement of the inner detector and muon spectrometer as explained in Section 4.2. The energy lost by an isolated muon in the calorimeters is not added to the calorimeter term. For a non-isolated muon, the energy lost in the calorimeter cannot be separated from the nearby jet energy. The muon spectrometer measurement of the muon momentum after energy loss in the calorimeter is therefore used unless there is a significant mis-match between the spectrometer and combined measurements, in which case the combined measurement minus the parameterised energy loss in the calorimeter is used. For higher values of the pseudorapidity outside the fiducial volume of the inner detector ( $2.5<|\eta|<2.7$ ), there is no matched track requirement and the muon spectrometer stand-alone measurement is used instead.

In both the electron and muon cases, the $E_{T}^{\text {miss }}$ is defined as:

$$
\begin{equation*}
E_{\mathrm{T}}^{m i s s}=\sqrt{\left(E_{x}^{m i s s}\right)^{2}+\left(E_{y}^{m i s s}\right)^{2}} \tag{4}
\end{equation*}
$$

The performance of the $E_{\mathrm{T}}^{\mathrm{miss}}$ reconstruction in minimum-bias data is described in Ref. [27].

## 5 Event selection and preparation

### 5.1 Event selection

The data presented in this note were collected over a ten-week period, from March to June 2010. From all data taken at a centre-of-mass energy of 7 TeV and for which the LHC declared stable beams, only
those with the detector high voltage in nominal condition are selected. Both the electron and muon channels require that all of the essential sub-detectors are operational such that the response and main criteria needed for particle identification as well as energy and momentum computations do not deviate significantly from their expected behaviour. In addition, while the electron channel analysis requires the solenoid to be on, the muon channel analysis needs both solenoid and toroid at nominal field. These basic data-quality requirements resulted in total integrated luminosities of $16.9 \mathrm{nb}^{-1}$ and $17.0 \mathrm{nb}^{-1}$ for the $W \rightarrow e v$ and $Z \rightarrow e e$ channels, respectively, and $16.6 \mathrm{nb}^{-1}$ and $17.7 \mathrm{nb}^{-1}$ for the $W \rightarrow \mu \nu$ and $Z \rightarrow \mu \mu$ channels, respectively. While the $W \rightarrow \mu \nu$ analysis requires calorimeter information to calculate the $E_{\mathrm{T}}^{\text {miss }}$, no calorimeter information used for the $Z \rightarrow \mu \mu$ channel. This is the reason why this channel does not have the same integrated luminosity as the electron channel. The uncertainty on the luminosity determination is estimated to be $11 \%$ [13].

Events are selected with the hardware-based L1 trigger. The L1 calorimeter trigger selects photons and electrons within $|\eta|<2.5$ using calorimeter information with the reduced granularity of trigger towers of dimension $\Delta \eta \times \Delta \phi=0.1 \times 0.1$. The calorimeter trigger used in this analysis accepts electron and photon candidates if the signal from a cluster of trigger towers is above five trigger counts, where one count corresponds to approximately 1 GeV . The L1 muon trigger searches for patterns of hits within $|\eta|<2.4$ consistent with high $-p_{\mathrm{T}}$ muons originating from the interaction region. The trigger logic is based on three trigger stations. The algorithm requires a coincidence of hits in the different trigger stations within a road, which tracks the path of a muon from the interaction point through the detector. The width of the road is related to the $p_{\mathrm{T}}$ threshold to be applied. The muon trigger used in this analysis corresponds to the lowest $p_{\mathrm{T}}$ threshold trigger which has a fully-opened road with a two-station time coincidence. As a result of these trigger decisions, $2.4 \times 10^{6}$ and $2.0 \times 10^{6}$ events are triggered in the electron and muon channels, respectively.

Collision candidates are selected by requiring a primary vertex with at least three tracks, consistent with the beam spot position. To reduce fake collision candidates from cosmic-ray or beam-halo events, the muon analysis requires the primary vertex position along the beam axis to be within 15 cm of the nominal position.

### 5.2 Event preparation

An analysis of a high statistics sample of minimum-bias events has shown that events can occasionally contain very localised high-energy calorimeter deposits not originating from the proton-proton collision, but e.g. from sporadic discharges in the hadronic end-cap calorimeter, and more rarely coherent noise in the electromagnetic calorimeter. Cosmic-ray muons undergoing a hard bremsstrahlung are also a potential source of localised energy deposits uncorrelated to the primary proton-proton collisions.

The occurrence of these events is very rare but can potentially impact significantly the $E_{\mathrm{T}}^{\text {miss }}$ measurement by creating high-energy tails [28]. To remove such events, dedicated cleaning requirements using reconstructed jets (with the anti- $k_{t}$ algorithm [29]) in a narrow cone of size $\Delta R=0.4$ have been developed using a minimum-bias event sample. It was verified that these criteria remove less than $0.1 \%$ of minimum-bias events, $0.004 \%$ of $W \rightarrow \ell v$, and $0.01 \%$ dijet events in Monte Carlo simulation.

For the electron channel only, the quality of the reconstruction of the energy deposited by the electron in the liquid argon calorimeter is assessed. The event is rejected if the candidate electromagnetic cluster is located in any problematic region of this detector: regions affected by major high-voltage problems, isolated cells producing a high noise signal or no signal at all, and electronic front-end boards not providing any output signal. These problems can cause extended dead regions in a given layer of the calorimeter, which may have an important impact on the energy reconstruction of the electron. The loss in acceptance due to these requirements is $4.8 \%$ for the $W$ channel and $10.5 \%$ for the $Z$ channel.


Figure 1: Calorimeter $E_{T}$ of the cluster (a), as well as $\eta(b)$ and $\phi(c)$ of electron candidates after preselection for data and Monte Carlo candidates broken down into the various signal and background components. The total number of Monte Carlo candidates is normalised to the number of observed data candidates. In Figure 1(a), the total QCD background is broken down into its constituents: hadrons misidentified as electrons, electrons from conversions, and electrons from semi-leptonic decays of heavy quarks.


Figure 2: Combined $p_{\mathrm{T}}(a), \eta(b)$, and $\phi(c)$ of muon candidates after preselection for data and Monte Carlo candidates broken down into the various signal and background components. The total number of Monte Carlo candidates is normalised to the number of observed data candidates.

## 6 Preselection of high transverse-energy leptons

A preselection of high transverse-energy electrons and muons is made. Electron candidates with the identification level "loose" according to the algorithm as described in Section 4.1 are required to have a cluster $E_{\mathrm{T}}>20 \mathrm{GeV}$ within the range $|\eta|<2.47$, excluding the transition region between the barrel and end-cap calorimeters $(1.37<|\eta|<1.52)$. Muon candidate events selected according to the algorithm described in Section 4.2 are required to have at least one combined muon with $p_{\mathrm{T}}>15 \mathrm{GeV}$ and a $p_{\mathrm{T}}$ as measured by the muon spectrometer greater than 10 GeV , within the range $|\eta|<2.4$. The difference between the inner-detector and muon-spectrometer $p_{\mathrm{T}}$, corrected for the mean energy loss in upstream material, is required to be less than 15 GeV to increase the robustness against track reconstruction mismatches. The difference between the $z$ position of the muon track extrapolated to the beam line and the $z$ coordinate of the primary vertex is required to be less than 1 cm .

Figures 1 and 2 show the kinematic properties of these electron and muon candidates, respectively,


Figure 3: $E_{\mathrm{T}}^{\mathrm{miss}}$ of electron (a) and muon (b) candidates after preselection for data and Monte Carlo candidates broken down into the various signal and background components. The total number of Monte Carlo candidates is normalised to the number of observed data candidates. In Figure 3(a), the total QCD background is broken down into its constituents: hadrons misidentified as electrons, electrons from conversions, and electrons from semi-leptonic decays of heavy quarks.
and compare these to the signal and background Monte Carlo samples described in Section 3. At this stage of the selection, the candidate events are dominated by QCD background. For the electron channel, Figure 1(a) shows this background consists mainly of conversion events and hadrons faking electrons. If these QCD Monte Carlo distributions are normalised to the total integrated luminosity of the data, the dijet Monte Carlo over-estimates the amount of background by a factor of approximately 2.6 for the electron channel and a factor of 1.7 for the muon channel. The Monte Carlo distributions in Figures 1 and 2 have been normalised to the total number of data events, taking into account these scale factors for the QCD background. It is to be noted that all data distributions in this note are given with statistical error bars only, corresponding to $68.3 \%$ confidence intervals unless otherwise stated. These distributions show reasonable agreement in shape between data and Monte Carlo simulation. More details on the properties of inclusive electrons and muons are given in Refs. [30] and [31].

Figure 3 shows the transverse missing energy normalised in the same fashion as for Figures 1 and 2. An excess of events around the expected signal region ( $E_{\mathrm{T}}^{\text {miss }} \sim 40 \mathrm{GeV}$ and above) compared to the background is already visible at this stage of the selection. The four highest- $E_{\mathrm{T}}^{\text {miss }}$ candidates in the muon channel are all events with jets.

## 7 Selection and observation of $W$ candidates

Additional requirements beyond those imposed in Section 6 are used to better discriminate $W \rightarrow \ell v$ events from background events. The electron identification level as described in Section 4.1 is increased to "tight" while the minimum muon combined $p_{\mathrm{T}}$ is increased to 20 GeV . Only the highest $p_{\mathrm{T}}$ lepton in the event is used. In the electron channel, events that would pass the $Z \rightarrow e e$ selection as given in Section 11 are vetoed. In the muon channel, $Z \rightarrow \mu \mu$ events, where one muon is outside the acceptance of the detector, fake a large $E_{T}^{\text {miss }}$ signature and hence can mimic a $W$-boson signal. Since those events have only one reconstructed muon track by construction, a veto for these events cannot be applied. It


Figure 4: $E_{\mathrm{T}}^{\mathrm{miss}}$ versus calorimeter-isolation parameter for electron candidates (a) and track-isolation parameter for muon candidates (b) after preselection plus the "tight" requirement for electrons and muon combined $p_{\mathrm{T}}>20 \mathrm{GeV}$.


Figure 5: $E_{\mathrm{T}}^{\text {miss }}$ of selected electron (a) and muon (b) candidates.
should be noted that the acceptance of the electromagnetic calorimeter goes up to $|\eta|=4.9$ in contrast to the muon spectrometer acceptance which is limited to $|\eta|=2.7$.

The use of an isolation parameter to enhance the expected signal has been considered in the muon and electron channels. However, separate isolation requirements must be considered for the electron and muon channels since the electron can undergo bremsstrahlung while a muon is primarily defined by its track. In addition, the EM calorimeter requirements for the electrons use variables which already provide some effective isolation.

A calorimeter-based isolation parameter defined as the total calorimeter transverse energy in a cone


Figure 6: $E_{\mathrm{T}}^{\text {miss }}$ versus the electron cluster $E_{\mathrm{T}}(a)$ and the muon $p_{\mathrm{T}}(b)$. For the purpose of this figure, the requirement of the muon $p_{T}$ is lowered to 15 GeV .


Figure 7: $E_{\mathrm{T}}^{\text {miss }}$ versus $m_{\mathrm{T}}$ of the lepton- $E_{\mathrm{T}}^{\text {miss }}$ system for the electron (a) and muon (b) channels.
of $\Delta R<0.3$ surrounding the candidate electron cluster which is then divided by the cluster $E_{\mathrm{T}}$ is considered for the electron channel. A track-based isolation for the muon channel defined as the sum of inner-detector transverse momenta within a cone $\Delta R<0.4\left(\sum p_{T}^{I D}\right)$ which is then divided by the total combined muon $p_{\mathrm{T}}$ is considered in the muon channel. The minimum- $p_{\mathrm{T}}$ used in the isolation requirement is 1 GeV . These isolation parameters are shown in Figure 4 and are plotted against the $E_{\mathrm{T}}^{\text {miss }}$ of the event. The isolation variable will be used in the electron analysis to make a data-driven estimate of the background contributions to the $W \rightarrow e v$ candidates; therefore, no form of isolation is explicitly applied in the electron-channel selection. An isolation requirement of $\sum p_{T}^{I D} / p_{T}<0.2$ is used in the


Figure 8: $m_{\mathrm{T}}$ of the electron- $E_{\mathrm{T}}^{\text {miss }}$ system without (a) and with (b) a requirement of $E_{\mathrm{T}}^{\mathrm{miss}}>25 \mathrm{GeV}$. In Figure 8(a), the total QCD background is broken down into its constituents: hadrons misidentified as electrons, electrons from conversions, and electrons from semi-leptonic decays of heavy quarks.


Figure 9: $m_{\mathrm{T}}$ of the muon- $E_{\mathrm{T}}^{\text {miss }}$ system without (a) and with (b) a requirement of $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$.
muon analysis given that, after all other selections are made to identify $W$ candidates, this requirement rejects over $84 \%$ of the expected QCD background while keeping $99 \%$ of signal events.

All further results shown in this section have passed the preselection requirements of Section 6, the "tight" requirement for electrons, the muon combined $p_{\mathrm{T}}>20 \mathrm{GeV}$, and the muon isolation requirement.

The last step of the signal selection is additional kinematic requirements applied to the $E_{\mathrm{T}}^{\text {miss }}$ of the

| Requirement | Number of <br> candidates |
| :--- | :---: |
| Triggered (Section 5) | $2.4 \times 10^{6}$ |
| Preselection (Section 6) | $5.1 \times 10^{3}$ |
| Tight electron (Section 4.1) | 177 |
| $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ | 49 |
| $m_{\mathrm{T}}>40 \mathrm{GeV}$ | 46 |

Table 2: Number of $W \rightarrow e v$ candidates in data remaining after each major requirement is applied.

| Requirement | Number of <br> candidates |
| :--- | :---: |
| Triggered (Section 5) | $2.0 \times 10^{6}$ |
| Preselection (Section 6) | 1155 |
| $p_{\mathrm{T}}>20 \mathrm{GeV}$ | 420 |
| $\sum p_{T}^{I D} / p_{T}<0.2$ | 186 |
| $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ | 77 |
| $m_{\mathrm{T}}>40 \mathrm{GeV}$ | 72 |

Table 3: Number of $W \rightarrow \mu \nu$ candidates in data remaining after each major requirement is applied.
event and the transverse mass $m_{\mathrm{T}}$ of the lepton- $E_{\mathrm{T}}^{\text {miss }}$ system defined as

$$
\begin{equation*}
m_{\mathrm{T}}=\sqrt{2 p_{\mathrm{T}}^{\ell} p_{\mathrm{T}}^{v}\left(1-\cos \left(\phi^{\ell}-\phi^{v}\right)\right)} \tag{5}
\end{equation*}
$$

where the measured $E_{\mathrm{T}}^{\mathrm{miss}}$ components in $(x, y)$ provide the neutrino information. All Monte Carlo distributions shown in this section have been normalised to integrated luminosities of $16.9 \mathrm{nb}^{-1}$ and $16.6 \mathrm{nb}^{-1}$, in the electron and muon channels, respectively, using the cross sections as given in Table 1. In addition, the QCD background contributions have been scaled by factors of $1 / 2.6$ and $1 / 1.7$ in the electron and muon channels, respectively, to account for the over-estimation of the dijet Monte Carlo sample described in Section 6.

Figure 5 shows the $E_{\mathrm{T}}^{\text {miss }}$ distribution of all electron and muon candidates passing the requirements described above. Both distributions indicate that applying a minimum requirement on $E_{\mathrm{T}}^{\text {miss }}$ would greatly enhance the $W$ signal over the expected background. This observation is also evident from the two-dimensional plot of $E_{\mathrm{T}}^{\text {miss }}$ versus electron cluster $E_{\mathrm{T}}$ and muon combined $p_{\mathrm{T}}$ shown in Figure 6. True $W \rightarrow \ell v$ events in the Monte Carlo are predominantly at high $E_{\mathrm{T}}^{\mathrm{miss}}$ due to the escaping neutrino in the event. Although some of the QCD background may also have neutrinos in their final state, these events mostly populate the regions of small $E_{\mathrm{T}}^{\mathrm{miss}}$.

The transverse mass of the lepton- $E_{\mathrm{T}}^{\mathrm{miss}}$ system is highly correlated to the $E_{\mathrm{T}}^{\mathrm{miss}}$ of the event as is demonstrated in Figure 7 which shows a two-dimensional plot of the $E_{\mathrm{T}}^{\text {miss }}-m_{\mathrm{T}}$ plane. Figures 8 and 9 show projections of Figure 7 where the $m_{\mathrm{T}}$ of the event is shown without and with a requirement of $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$. In the muon channel, the events at very low- $m_{\mathrm{T}}$ have, in the transverse plane, their $E_{\mathrm{T}}^{\mathrm{miss}}$ direction aligned with that of the muon candidate.

Tables 2 and 3 summarise the number of $W \rightarrow \ell v$ candidates remaining after each major requirement in the respective analyses described in this note. A total of 46 candidates ( $27 e^{+}$and $19 e^{-}$) pass all requirements in the electron channel and 72 candidates ( $47 \mu^{+}$and $25 \mu^{-}$) in the muon channel in the $m_{\mathrm{T}}$ region above 40 GeV .


Figure 10: Pseudorapidity distributions of $e^{+}(a), e^{-}(b), \mu^{+}(c)$, and $\mu^{-}(d)$ candidates satisfying all $W$ requirements. The data describe well the larger expected fraction of $\ell^{+}$candidates at high pseudorapidity compared to $\ell^{-}$ due to the larger average rapidity of $W^{+}$bosons expected in proton-proton collisions.


Figure 11: Electron cluster $E_{T}(a)$ and muon $p_{T}(b)$ of the $W$ candidates after final selection. $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ and $m_{\mathrm{T}}>40 \mathrm{GeV}$ are required in both channels.


Figure 12: $\quad p_{\mathrm{T}}$ of the $W$ candidates in the electron-channel (a) and muon-channel (b) after final selection. $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ and $m_{\mathrm{T}}>40 \mathrm{GeV}$ are required in both channels.

## 8 Properties of $W \rightarrow \ell v$ candidates

For the final selection, the preselection requirements of Section 6, the "tight" requirement for electrons, the muon $p_{\mathrm{T}}>20 \mathrm{GeV}$ and muon isolation requirements, $E_{\mathrm{T}}^{\text {miss }}>25 \mathrm{GeV}$ and $m_{\mathrm{T}}>40 \mathrm{GeV}$ are used. Figure 10 shows the pseudorapidity distributions of the $\ell^{+}$and $\ell^{-}$candidate events that pass the final selection requirements. The larger expected fraction of $\ell^{+}$candidates at high pseudorapidity compared to $\ell^{-}$reflects the larger average rapidity of $W^{+}$bosons expected in proton-proton collisions. This is the motivation of the asymmetry measurement presented in Section 10.6 and so Figure 10 uses the $\eta$


Figure 13: (a) Calorimeter isolation variable divided by $E_{\mathrm{T}}$ (as described in Section 7) after preselection. The total number of Monte Carlo candidates is normalised to the number of observed data candidates. (b) Result of the template fit used to obtain an estimate of the QCD background, where the "tight" electron identification requirement has been substituted by "loose" to increase statistics (see text for details). The Monte Carlo distributions are scaled to the result of the fit.
binning of this measurement. Figure 11 shows the electron cluster $E_{T}$ and muon combined $p_{\mathrm{T}}$ of the lepton candidates while Figure 12 shows the $p_{\mathrm{T}}$ spectrum of the $W \rightarrow \ell v$ candidates. Both channels demonstrate a clear $W$ signal over an almost negligible background.

## 9 Background expectations for the $W \rightarrow \ell v$ candidates

The Monte Carlo samples discussed in Section 3 are used to provide an expectation for signal events and, in some cases, for the background events. The QCD component of the background is estimated from the data (as discussed below) while the electroweak component of the background is obtained from the appropriate Monte Carlo samples. The numbers of observed candidates and expected background events in both channels are summarised in Table 4. The difference between the expectations for the electron and muon channels stem primarily from the lower reconstruction efficiency of "tight" electrons compared to that of combined muons.

### 9.1 Background estimation for the electron channel

For the electron channel, the contribution from the $W \rightarrow \tau \nu$ process is expected to be small (1.4 events) and the contribution from $Z \rightarrow e e$ decays even smaller ( 0.1 events). The QCD background expectation is divided between heavy-quark decays, conversions, and hadrons faking electrons. A partially data-driven estimate of the QCD background to the observed $W$ candidate events is made. The calorimeter isolation in a cone of $\Delta R=0.3$ divided by the electron $E_{\mathrm{T}}$ (as described in Section 7) is used as a discriminating variable in a binned maximum likelihood fit. This technique uses the prediction for the shape of the signal and the QCD background for this variable in the form of histogram templates taken from Monte Carlo samples. The distribution of this variable after the preselection is shown in Figure 13(a).

Due to the limited statistics and the very few background events, the fit cannot be performed after


Figure 14: Track-isolation variable $\sum p_{T}^{I D} / p_{T}$ (a) and $E_{\mathrm{T}}^{\text {miss }}$ distribution of events in the control region (see text) (b) after muon preselection (only QCD background is shown). The total number of Monte Carlo candidates is normalised to the number of observed data candidates.
the final selection. Therefore only the "loose" instead of the "tight" electron identification requirement as described in Section 4.1 is applied, while the requirements on $E_{\mathrm{T}}^{\text {miss }}$ and $m_{\mathrm{T}}$ are kept. Also for this reason, the signal and background templates are obtained from Monte Carlo samples. The fit result is shown in Figure 13(b) and provides a background estimate of $N_{\mathrm{QCD}}$ loose $=40.6 \pm 8.0$ events, where the uncertainty contains the statistical uncertainty of the data and of the templates. The number of QCD background events after the final selection is estimated by scaling this number with the jet rejection factor for the "tight" requirement, with respect to the "loose" requirement. The central value of the rejection factor is extracted from Monte Carlo, while its systematic uncertainty is estimated by comparing Monte Carlo and data rejection factors, obtained in five low $E_{\mathrm{T}}^{\text {miss }}$ bins of 5 GeV between $0-25 \mathrm{GeV}$ with small signal contribution. The rejection factor, quoted here as its reciprocal, is found to be $0.03 \pm 0.01$, giving a total QCD background of $N_{\mathrm{QCD}}$, tight $=1.1 \pm 0.2$ (stat). The total background in the electron channel is estimated to be this QCD contribution plus that coming from the $W \rightarrow \tau v$ (1.4 events) and $Z \rightarrow e e$ ( 0.1 events) processes.

Various sources of systematic uncertainties were investigated. The QCD PYTHIA template was replaced by one obtained from data using the "loose" selection without $E_{\mathrm{T}}^{\text {miss }}$ and $m_{\mathrm{T}}$ cut. In addition, instead of dropping the "tight" requirement, the fit was performed on a sample where the "tight" requirement was applied but the $E_{\mathrm{T}}^{\text {miss }}$ and $m_{\mathrm{T}}$ requirements were dropped. The observed variations are all small compared to the uncertainty due to the tight-to-loose rejection factor. Therefore, the number of QCD background events as estimated by this template method is $N_{\mathrm{QCD}}=1.1 \pm 0.2$ (stat) $\pm 0.4$ (syst). The predicted number of QCD background events based on the dijet Monte Carlo and scaled by the factor of $1 / 2.6$ (as described in Section 6) is $0.7 \pm 0.2$ (stat) events and so is in agreement with this measurement. These estimates for the QCD background contribution to the $W$ channel will greatly benefit from more statistics.

### 9.2 Background estimation for the muon channel

For the muon channel, the total background estimate is 5.3 events, primarily coming from $Z \rightarrow \mu \mu$ and $W \rightarrow \tau \nu$ decays, respectively $42 \%$ ( $2.23 \pm 0.16$ events) and $36 \%$ ( $1.90 \pm 0.13$ events) of all the background. Background from multijets is $16 \%$ and the remaining $6 \%$ comes from top production ( $4.5 \%$ ) and from $Z \rightarrow \tau \tau$ decay ( $1.5 \%$ ). Given the high uncertainty in the Monte Carlo dijet cross section, this source of background has been measured in data using the distribution of transverse missing energy versus isolation prior to the transverse mass requirement, as described below. The isolation distribution for preselected events is shown in Figure 14(a).

The primary assumption of this method to extract the multijet component of the total background is that the $E_{\mathrm{T}}^{\text {miss }}$ and the lepton isolation are uncorrelated. The $E_{\mathrm{T}}^{\text {miss }}$ versus track-isolation plane is divided into four separate regions defined by the $E_{\mathrm{T}}^{\text {miss }}$ and isolation requirements as for the $W$ selection (Figure 4(b)). The background contribution to the $W$ signal region is obtained from a similarity relationship between the contents in the four regions of the $E_{\mathrm{T}}^{\text {miss }}$-isolation space [32]. The calculation is corrected for the contributions from the signal and the electroweak backgrounds outlined above.

The background estimation method described above yields a jet background estimate of $3.8 \pm 1.3$ events if no $m_{\mathrm{T}}$ requirement is imposed, which corresponds to $0.9 \pm 0.3$ (stat) $\pm 0.6$ (syst) events if $m_{\mathrm{T}}>40 \mathrm{GeV}$. The systematic uncertainty in this method is due to the correlation between the two variables used and it has been estimated in a consistency check applying the same technique on a Monte Carlo QCD sample. A 70\% systematic uncertainty is estimated from the difference between the number of predicted events from Monte Carlo and the number of observed events in the signal region in data. This technique provides the better estimation of the background in multijet events because it is also sensitive to poorly reconstructed events faking muons as well as pion and kaon decays and so is used as the default for this analysis, rather than the alternate method discussed immediately below.

An alternative estimation of the multijet background has been made by measuring the QCD background normalisation in data. The control sample used is obtained by reversing the isolation requirement after preselection. The assumption is that these events are dominated by muons from QCD background events. The background normalisation is taken from the comparison of the distributions of $E_{\mathrm{T}}^{\text {miss }}$, in both data and jet background Monte Carlo samples. These are shown in Figure 14(b), where the QCD background distribution has been normalised to the numbers of events in the control sample. The data and Monte Carlo shapes agree well and an overall scale factor of Monte Carlo QCD cross section to data of $0.58 \pm 0.05$ (stat) is measured as described in Section 3. This method derives a QCD background estimate of $0.28 \pm 0.05$ (stat). A value in agreement with this estimate is found when decreasing the muon transverse momentum requirement to 15 GeV (in order to get more statistics). A study using dijet Monte Carlo predicts that the background contamination from pion and kaon decays is $0.45 \pm 0.45$ (tot), which is within the direct estimation from data.

All muon candidate events were inspected individually, verifying the main reconstruction parameters. Distributions of hit multiplicities in inner-detector and muon-spectrometer tracks, their track-matching $\chi^{2}$, and the difference in the transverse momentum measurement between the two sub-detectors were compared in data and Monte Carlo. Good agreement was found for all of these items. The hypothesis that a cosmic ray overlays with the collision was carefully examined by looking at the timing properties of muon tracks. TRT, tile calorimeter and MDT time measurements were analysed and no indication of cosmic contamination was found.

Detailed estimates of uncertainties in these backgrounds due to the statistically limited control samples and Monte Carlo simulations, and also from leading-order jet cross sections and fragmentation functions will be evaluated in future studies with higher data statistics.

| $\ell$ | Observed <br> candidates | Background <br> $(\mathrm{EW})$ | Background <br> $(\mathrm{QCD})$ | Background-subtracted <br> signal $N_{W}^{\text {sig }}$ |
| :---: | :---: | :---: | :---: | :---: |
| $e^{+}$ | 27 | $0.9 \pm 0.0 \pm 0.1$ | $0.6 \pm 0.1 \pm 0.3$ | $25.6 \pm 5.2 \pm 0.3$ |
| $e^{-}$ | 19 | $0.6 \pm 0.0 \pm 0.1$ | $0.6 \pm 0.1 \pm 0.3$ | $17.8 \pm 4.4 \pm 0.3$ |
| $e^{ \pm}$ | 46 | $1.5 \pm 0.0 \pm 0.1$ | $1.1 \pm 0.2 \pm 0.4$ | $43.4 \pm 6.8 \pm 0.4$ |
| $\mu^{+}$ | 47 | $2.4 \pm 0.0 \pm 0.2$ | $0.7 \pm 0.3 \pm 0.5$ | $43.8 \pm 6.9 \pm 0.6$ |
| $\mu^{-}$ | 25 | $2.0 \pm 0.0 \pm 0.2$ | $0.2 \pm 0.1 \pm 0.2$ | $22.8 \pm 5.0 \pm 0.3$ |
| $\mu^{ \pm}$ | 72 | $4.4 \pm 0.0 \pm 0.3$ | $0.9 \pm 0.3 \pm 0.6$ | $66.7 \pm 8.5 \pm 0.7$ |

Table 4: Numbers of observed candidate events for the $W \rightarrow \ell v$ channel, electroweak (EW) and dataderived QCD background events, and background-subtracted signal events. The first uncertainty is statistical (signal statistical uncertainties are described in Section 10 while Monte Carlo statistical errors are negligible). The second uncertainty represents the systematics (as described in the text). In addition to what is quoted in this table, an $11 \%$ uncertainty on the luminosity determination is applicable to the electroweak background.

### 9.3 Observed candidate events

Table 4 summarises the numbers of observed candidate events for the $W \rightarrow \ell v$ channel, the number of background events from both the QCD and electroweak processes, and the number of backgroundsubtracted signal events. The first uncertainty is due to statistics and is described in Section 10. Monte Carlo statistical uncertainties are considered to be negligible in comparison to the statistical uncertainties associated to the data and to the estimation of the QCD background. The second uncertainty is a systematic one. For the electron (muon) electroweak background, this amounts to the $5 \%$ ( $7 \%$ ) experimental systematic uncertainty (Section 10.2.1), $4 \%$ systematic uncertainty on the predicted cross section (Section 3), and $3 \%$ on the parton distribution function acceptance (Section 10.3) resulting in a total systematic uncertainty of $7 \%$ ( $8 \%$ ) for the electron (muon) channel. The QCD background systematic uncertainties are explained in this section. The luminosity determination uncertainty of $11 \%$ is used in both channels but is only applicable to the electroweak background. The numbers in Table 4 form the basis of the cross section measurements and the $W$ asymmetry measurements presented in Section 10.

## 10 Cross-section measurements for $W$-boson decays to electrons and muons

### 10.1 Introduction

The $W$-boson cross-section measurement is given by:

$$
\begin{equation*}
\sigma_{t o t}=\sigma_{W} \times B R(W \rightarrow \ell v)=\frac{N_{W}^{s i g}}{A_{W} C_{W} L_{i n t}} \tag{6}
\end{equation*}
$$

where

- $N_{W}^{s i g}$ denotes the number of background-subtracted signal events in the channel of interest, as summarised in Table 4;
- $A_{W}$ denotes the so-called geometrical acceptance for the $W$-boson decays under consideration, defined as the fraction of decays satisfying the geometrical and kinematical (fiducial) constraints at
the generator level. These include the $\eta$ requirements as given in Section 6, as well as requirements on $p_{\mathrm{T}}{ }^{\ell}>20 \mathrm{GeV}, p_{\mathrm{T}}{ }^{\nu}>25 \mathrm{GeV}$, and $m_{\mathrm{T}}>40 \mathrm{GeV}$ at the generator level. This quantity can only be determined from $W \rightarrow \ell v$ Monte Carlo simulation at generator level;
- $C_{W}$ denotes the ratio between number of signal events which pass the final selection requirements after reconstruction and the total number of generated events within the fiducial volume. In this note, $C_{W}$ is estimated using Monte Carlo signal simulation, but this correction factor includes the efficiency for triggering on lepton candidates as well as reconstructing/identifying $W$-boson decays falling within the geometrical acceptance. The different components of $C_{W}$ can be estimated using Monte Carlo simulation but most of these will eventually be determined from data-driven measurements. In this note, the correction factors $C_{W}$ are fully taken from simulation for the electron channel, but some data-driven corrections are used for the muon channel, as described in Section 10.2.2;
- and $L_{i n t}$ denotes the integrated luminosity for the channel of interest.

The geometrical acceptance $A_{W}$, as well as the denominator of $C_{W}$, are computed at the Born level, i.e. from lepton kinematics before QED radiation. The factor $C_{W}$ thus includes the corrections for the QED final state radiation.

Equation 6 defines the measured total inclusive cross sections for each channel, $\sigma_{t o t}$. Equation 6 with the geometrical acceptance $A_{W}$ set to unity defines the measured fiducial inclusive cross sections $\sigma_{\text {fid }}$ for each channel. These fiducial cross sections do not rely strongly on any theoretical prediction for the geometrical acceptance and therefore do not contain significant theoretical uncertainties related to it. Cross-section results in this note will be presented for both the electron and muon channels, separated by and averaged over charges.

The Eq. 6 above assumes that only one correction factor $C_{W}$ is needed for the fiducial cross-section calculation. This specific case can be interpreted as a cross-section measurement in phase space defined by the fiducial requirements at Monte Carlo truth level. This simplified approach is biased where the predicted kinematical distributions of the $W$-bosons entering $C_{W}$ via the signal simulation differ from reality. This bias has been checked to be negligible compared to the statistical uncertainties of the measurements presented here (see Figures 11 and 12 which demonstrate the agreement between data and Monte Carlo simulation for various kinematic distributions). For the electron channel, a large number of pseudo-experiments binned, in $E_{\mathrm{T}}$ and $\eta$, corresponding to the statistics observed in the electron channel has been performed to verify that the biases of the single bin approach are negligible (below the percent level).

In the following, the efficiencies and correction factors with their associated experimental systematic uncertainties are discussed separately for the electrons and muons. The fiducial and total cross sections are derived next with their associated statistical, experimental systematic, and luminosity uncertainties. These results are compared to the most recent theoretical calculations. In the final part of this section, the measured lepton asymmetry in the fiducial acceptance is also presented.

### 10.2 Detector-related efficiencies/scale factors and the uncertainty on $C_{W}$

The primary components of the correction factor $C_{W}$ shown in Eq. 6 come from the detector-related efficiencies such as triggering and reconstruction/identification of leptons. These values and their uncertainties feed directly into the determination of the cross section. These efficiencies are summarised in Table 5 for the electron channel and in Table 6 for the muon channel and are further described below. The final values for $C_{W}$ will later be presented in Table 8.

For the case of the muon channel, differences were observed between data and Monte Carlo for some of these efficiency values. For this reason, additional data-derived scale factors are applied to the

| Electron channel |  |
| :--- | :---: |
| Trigger efficiency | $0.999 \pm 0.001$ (tot) |
| Reconstruction/identification efficiency | $0.78 \pm 0.05$ (syst) |

Table 5: Detector-related efficiencies used in the extraction of the measured cross sections for the electron channel. No scale factor to correct the Monte Carlo sample are used in this channel.

| Muon channel |  |
| :--- | :---: |
| Trigger efficiency | $0.88 \pm 0.01 \pm 0.03$ |
| Reconstruction/identification efficiency | $0.97 \pm 0.01 \pm 0.04$ |
| Trigger scale factor | $0.97 \pm 0.01 \pm 0.04$ |
| Reconstruction scale factor | $0.99 \pm 0.01 \pm 0.04$ |

Table 6: Detector-related efficiencies after all corrections used in the extraction of the measured cross sections for the muon channel. The data-derived scale factors were used to correct the Monte Carlo sample to the data value. The first uncertainty is statistical and the second is systematic.

Monte Carlo sample. These scale factors are also presented in Table 6 and described below. No such correction factors are applied to the electron channel, where the trigger efficiency agrees between data and Monte Carlo, and reconstruction/identification of leptons cannot yet be measured from data due to lack of high- $E_{\mathrm{T}}$-electron statistics.

### 10.2.1 Electron efficiencies and systematic uncertainty on $C_{W}$

The most important efficiency component for the electron channel is the tight electron reconstruction and identification efficiency measured with respect to all reconstructed electron candidates. Its average value is $78 \%$. This efficiency depends strongly on both $E_{\mathrm{T}}$ and $\eta$ of the electron. Most of this dependence arises from material interactions in the inner detector and is a significant source of systematic uncertainty as discussed below. A total systematic uncertainty of $\pm 6 \%$ is assigned to the tight electron identification efficiency and comes from these material effects as well as observed discrepancies in the electron identification variables, as mentioned below.

It should be noted that the performance-based efficiency definition discussed in Section 4.1 leads to a tight electron efficiency which is $6 \%$ lower than the one determined by truth-matching the reconstructed electron to the $W$, as used in this cross-section determination ( $78 \%$ ). This change of definition for efficiency is consistently taken into account in the calculation of $C_{W}$, which is derived for the $W$-matched tight electrons. This choice of definition for the tight electron identification efficiency is one of the largest contributors to the difference between the electron efficiency value of $78 \%$ and the final value for $C_{W}$ value quoted below.

The correction factor $C_{W}$ that feeds directly into the cross-section Eq. 6 includes as a primary component the efficiency for reconstructing and identifying $W$-boson decays falling within the geometrical acceptance. The tight electron identification efficiency mentioned above is calculated with respect to all reconstructed candidate electrons and so additional factors must be taken into account for electrons that are in the acceptance but, due to various effects, fail to even be reconstructed as candidate electrons. An important source of loss is the fiducial selection of the approximately $5 \%$ problematic regions of the calorimeter as specified in Section 5.2 and an additional $5 \%$ loss due to the kinematic and $E_{\mathrm{T}}$ requirements. The correction factor $C_{W}$ in addition accounts for inefficiencies for selecting collisions with a reconstructed vertex (a minor contribution), and also includes contributions from trigger effects as well
as electron energy and $E_{\mathrm{T}}^{\text {miss }}$ scale and resolutions, as explained below. The total systematic uncertainty on $C_{W}$ is then the quadratic sum of the following contributions:

- Trigger efficiency: The trigger efficiency has been measured in data to be better than $99.9 \%$, and carries a negligible statistical and systematic uncertainty;
- Discrepancies in electron identification variables: Such discrepancies in electron identification variables have been observed for both electron and photon candidates in samples, however, contaminated by significant background [22]. A systematic uncertainty was obtained by varying the observed shapes for the Monte Carlo signal electrons from $W$-boson decay to match those observed for electron candidates in the same kinematic range in data. A systematic uncertainty of $\pm 6 \%$ is assigned to $C_{W}$.
- Material effects and problematic regions in the calorimeter: The impact of possible extra material in the inner detector and in front of the active EM calorimeter has been evaluated with a dedicated simulation. There are two components that contribute to the overall systematic uncertainty due to this effect: impact on the reconstruction of candidate electrons and on the tight electron identification efficiency. An additional smaller uncertainty is attributed to electrons that fail to be reconstructed due to problematic regions in the liquid argon calorimeter. A total systematic uncertainty of $\pm 4 \%$ is assigned to $C_{W}$;
- Energy scale and resolution: The impact of the electron scale and resolution is dominated by the estimated uncertainty on the EM calorimeter energy scale of $\pm 3 \%$ based on test-beam measurements and first in-situ measurements of $\pi^{0} \rightarrow \gamma \gamma$ [33]. Varying the energy scale by this factor (which includes the proper recalculation of $E_{\mathrm{T}}^{\text {miss }}$ ) provides an uncertainty of $\pm 3 \%$ on $C_{W}$;
- $E_{\mathrm{T}}^{\text {miss }}$ scale and resolution: Several possible sources of uncertainty on the $E_{\mathrm{T}}^{\text {miss }}$ scale and resolution have been considered such as the energy scale of the clustering algorithm used in the construction of $E_{\mathrm{T}}^{\text {miss }}$ variable [34], the impact of pile-up in the data sample, and the problematic regions in the calorimeter, resulting in an estimated uncertainty of $\pm 2 \%$ on $C_{W}$.

In summary, the final $C_{W}$, averaged over all bins in electron $\eta$ and $E_{\mathrm{T}}$, is 0.656 with a total systematic uncertainty of $\pm 8 \%$.

### 10.2.2 Muon efficiencies, scale factors, and uncertainty on $C_{W}$

Several important components such as muon reconstruction and trigger efficiencies feed into the evaluation of $C_{W}$ and its systematic uncertainty. These efficiencies have been measured in Monte Carlo and corrected by data-driven scale factors to take into account differences between data and simulation. The numbers used in the cross section calculation and the measured scale factors are presented in Table 6.

The muon reconstruction efficiency as determined from the Monte Carlo and corrected by the scale factor is $0.97 \pm 0.01$ (stat) $\pm 0.04$ (syst). The scale factor of $0.99 \pm 0.01$ (stat) $\pm 0.04$ (syst) was obtained from efficiency studies of isolated combined muon tracks relative to inner detector tracks matched to muon hits in the muon spectrometer which reduce the contribution of fake muons. The inner-detector track efficiency and the muon hit efficiency are considered well modelled in the Monte Carlo, and a systematic is assigned to the level of agreement of this assumption.

The trigger efficiency of $0.88 \pm 0.01$ (stat) $\pm 0.03$ (syst) was obtained by correcting the value obtianed in Monte Carlo with the correction factor of $0.97 \pm 0.01$ (stat) $\pm 0.04$ (syst) measured from data. This has been derived by comparing the relative trigger efficiency for reconstructed muons above 15 GeV in data and simulations for both barrel and end-cap trigger systems.

The systematic uncertainty on $C_{W}$ comes in part from the uncertainties on the reconstruction and trigger efficiencies mentioned above. Other effects are due to inefficiencies for selecting collisions with a reconstructed vertex (a minor contribution), as well as the muon and $E_{\mathrm{T}}^{\mathrm{miss}}$ energy scale and resolutions. The total systematic uncertainty on $C_{W}$ is then the quadratic sum of the following contributions:

- Muon reconstruction: This systematic uncertainty of $\pm 4 \%$ is dominated by the dependence of the efficiency on the transverse momenta and the uncertainty on the remaining $\pi / \mathrm{K}$ contamination in the data sample where the efficiency is measured;
- Trigger efficiency: This uncertainty of $\pm 4 \%$ is derived by changing the tolerance on the matching between tracks and trigger signals and comparing measurements obtained in different trigger data streams. This number is a weighted average of the RPC and TGC trigger efficiency uncertainties (respectively $\pm 5 \%$ and $\pm 3 \%$ );
- Energy scale and resolution: This uncertainty estimation is obtained by applying a smearing of Monte Carlo muon momentum resolution and scale using parameters in agreement with the data ( $5 \%$ in the barrel and $8.5 \%$ in the endcap for the resolution and $2 \%$ for the scale) [23]. A systematic uncertainty of $\pm 4 \%$ is assigned to $C_{W}$.
- $E_{\mathrm{T}}^{\text {miss }}$ scale and resolution: Several possible sources of uncertainty on the $E_{\mathrm{T}}^{\text {miss }}$ scale and resolution have been considered as discussed Section 10.2.1, resulting in an estimated uncertainty of $\pm 2 \%$ on $C_{W}$.

The final $C_{W}$ is 0.814 with a total systematic uncertainty of $\pm 7 \%$.

### 10.3 Geometrical acceptance and uncertainty

The calculation of the total cross section takes into account the phase-space requirements applied in the fiducial cross-section measurement and is entirely based on Monte-Carlo simulations. This geometrical acceptance factor, $A_{W}$, is defined as

$$
\begin{equation*}
A_{W}=\left(\frac{N^{a c c}}{N^{a l l}}\right)_{g e n} \tag{7}
\end{equation*}
$$

where $N^{a c c}$ is the number of generated events that pass the fiducial requirements (accepted events as defined in Sections 6 and 7) and $N^{\text {all }}$ is the total number of generated events at truth level. The quantity $A_{W}$ is determined at Born level, i.e. before the decay lepton may emit photons (QED final-state radiation) and the losses due to this effect become a component of the $C_{W}$, evaluated with the full simulation of the detector response.

The acceptance is calculated using the PYTHIA $W$ samples generated with the modified LO parton distribution function (PDF) MRSTLO* [16] and the corresponding ATLAS MC09 tune [35]. The central values of the acceptances are provided in Table 7. The statistical uncertainty resulting from the Monte Carlo sample is negligible.

The systematic uncertainties on the acceptance are dominated by the limited knowledge of the proton PDFs and the modelling of the $W$-production at the LHC. These uncertainties are evaluated using dedicated MC@NLO [36] samples generated with two different NLO PDFs: the CTEQ6.6 PDF [37] and HERAPDF1.0 [38]. The latter predicts a noticably higher $W^{+}\left(W^{-}\right)$cross section by $1.7 \%$ ( $4.4 \%$ ) and, for this reason, is a good choice to use as one of the alternative samples for the evaluation of the systematic uncertainty. The acceptance results determined with these alternate PDFs are presented in Table 7.

The systematic uncertainty on the acceptance is derived from the following two sources:

| MC | $A_{W}$ <br> $W^{+} \rightarrow e^{+} v$ | $A_{W}$ <br> $W^{+} \rightarrow \mu^{+} v$ | $A_{W}$ <br> $W^{-} \rightarrow e^{-} v$ | $A_{W}$ <br> $W^{-} \rightarrow \mu^{-} v$ | $A_{W}$ <br> $W \rightarrow e v$ | $A_{W}$ <br> $W$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| PYTHIA MRSTLO* | 0.466 | 0.484 | 0.457 | 0.475 | 0.462 | 0.480 |
| MC@NLO HERAPDF1.0 | 0.475 | 0.494 | 0.454 | 0.472 | 0.465 | 0.483 |
| MC@NLO CTEQ6.6 | 0.478 | 0.496 | 0.452 | 0.470 | 0.465 | 0.483 |

Table 7: Summary of geometrical acceptance values $A_{W}$ for $W \rightarrow e v$ and $W \rightarrow \mu \nu$ using various MonteCarlo simulations.

- The difference for the MC@NLO geometrical acceptances using the two PDFs is at most $\pm 0.6 \%$ while the statistical precision per sample is negligible. The relative uncertainties, estimated by using the CTEQ6.6 PDF error eigenvector sets at the $90 \%$ C.L. limit, in combination with the MC@NLO acceptance calculation, are $\pm 1.0 \%$ for the $W^{+}$and $\pm 1.8 \%$ for the $W^{-}$production.
- The geometrical acceptances obtained with MC@NLO are larger by $2.6 \%(2.1 \%)$ and smaller by $1.1 \%(1.1 \%)$ for $W^{+}$and $W^{-}$production in the electron channel (muon channel), respectively, when compared to the PYTHIA values.

These two components added in quadrature result in systematic uncertainties on the acceptance values for $W^{+}$and $W^{-}$production of approximately $\pm 3 \%$ and $\pm 2 \%$, respectively. Given that only two alternate PDFs were used to illustrate the possible range of this uncertainty, the more conservative of these two values, $\pm 3 \%$, is used as the overall relative systematic uncertainty for the PYTHIA acceptance values. This value is dominated by the large difference to the MC@NLO values.

### 10.4 Measured cross sections

All of the elements necessary to calculate the fiducial and total cross sections for $W^{+}, W^{-}$, and $W^{ \pm}$production and decay in the electron and muon channels are summarised in Table 8. The derived fiducial and total cross sections are also presented in this table, along with their statistical, systematic and luminosity uncertainties. The total cross section values for the combined electron-muon channels, when taking into account the correlated and uncorrelated sources of uncertainty, are $\sigma_{\text {tot }}\left(W^{+}\right)=$ $[5.7 \pm 0.7$ (stat) $\pm 0.4($ syst $) \pm 0.6($ lumi $)] \mathrm{nb}, \sigma_{\text {tot }}\left(W^{-}\right)=[3.5 \pm 0.5$ (stat) $\pm 0.2($ syst $) \pm 0.4$ (lumi) nb , and $\sigma_{\text {tot }}\left(W^{ \pm}\right)=[9.3 \pm 0.9($ stat $) \pm 0.6($ syst $) \pm 1.0($ lumi $)] \mathrm{nb}$.

### 10.5 Comparison to theoretical calculations

A comparison of the measured cross-section values to theoretical predictions including next-to-next-toleading order QCD corrections is shown in Figure 15 (where the electron and muon channels are shown separately) and Figure 16 (where the electron and muon channels are combined). The calculations were performed with the program FEWZ [18] using the MSTW2008 NNLO structure function parameterisation [19]. The renormalisation scale $\mu_{R}$ and factorisation scale $\mu_{F}$ were chosen to be $\mu_{F}=\mu_{R}=m_{W}$. Within the experimental uncertainties, the measured cross sections agree well with the calculations for both $W^{+}$and $W^{-}$production and the expected asymmetry between these cross sections is confirmed experimentally. It should be noted that the theoretical uncertainties resulting from variations of the renormalisation and factorisation scales as well as uncertainties resulting from structure-function parameterisations are not shown. As discussed in Section 3, these uncertainties are expected to be of the order of $\pm 4 \%$ at 7 TeV . Figure 15 also displays the results of previous measurements of the total $W$ production cross section by the CDF [7] and D0 [6] experiments at $\sqrt{s}=1.96 \mathrm{TeV}$ at the Fermilab Tevatron collider and by the UA1 [39] and UA2 [40] experiments at $\sqrt{s}=0.63 \mathrm{TeV}$ at the CERN Sp $\overline{\mathrm{p} S}$ protonantiproton collider. All measurements are in good agreement with the theoretical prediction. The energy dependence of the total $W$-production cross section is well described.

|  | $W^{+}$ |  |  |  | $W^{-}$ |  |  |  | $W^{ \pm}$ |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Electron channel |  |  |  |  |  |  |  |  |  |  |  |  |
|  | value | stat | syst | lumi | value | stat | syst | lumi | value | stat | syst | lumi |
| Backgroundsubtracted signal | 25.6 | 5.2 | 0.3 | 0.1 | 17.8 | 4.4 | 0.3 | 0.1 | 43.4 | 6.8 | 0.4 | 0.2 |
| Correction $C_{W}$ | 0.653 | - | 0.052 | - | 0.660 | - | 0.053 | - | 0.656 | - | 0.053 | - |
| Fiducial cross section (nb) | 2.3 | 0.5 | 0.2 | 0.3 | 1.6 | 0.4 | 0.1 | 0.2 | 3.9 | 0.6 | 0.3 | 0.4 |
| Acceptance $A_{W}$ | 0.466 | - | 0.014 | - | 0.457 | - | 0.014 | - | 0.462 | - | 0.014 | - |
| Total cross section (nb) | 5.0 | 1.0 | 0.4 | 0.5 | 3.5 | 0.9 | 0.3 | 0.4 | 8.5 | 1.3 | 0.7 | 0.9 |
| Muon channel |  |  |  |  |  |  |  |  |  |  |  |  |
|  | value | stat | syst | lumi | value | stat | syst | lumi | value | stat | syst | lumi |
| Backgroundsubtracted signal | 43.8 | 6.9 | 0.6 | 0.3 | 22.8 | 5.0 | 0.3 | 0.2 | 66.7 | 8.5 | 0.7 | 0.5 |
| Correction $C_{W}$ | 0.822 | - | 0.057 | - | 0.804 | - | 0.057 | - | 0.814 | - | 0.056 | - |
| Fiducial cross section (nb) | 3.2 | 0.5 | 0.2 | 0.4 | 1.7 | 0.4 | 0.1 | 0.2 | 4.9 | 0.6 | 0.4 | 0.5 |
| Acceptance $A_{W}$ | 0.484 | - | 0.014 | - | 0.475 | - | 0.014 | - | 0.480 | - | 0.014 | - |
| Total cross section (nb) | 6.6 | 1.0 | 0.5 | 0.7 | 3.6 | 0.8 | 0.3 | 0.4 | 10.3 | 1.3 | 0.8 | 1.1 |

Table 8: Results for the fiducial cross sections $\sigma_{\text {fid }}$ and total cross section $\sigma_{\text {tot }}$ for $W^{+}, W^{-}$, and $W^{ \pm}$in the electron and muon channels. Shown are the observed numbers of signal events after background subtraction for each channel, the average correction factors $C_{W}$, the fiducial cross sections, the geometrical acceptance correction factors, and the total cross sections with their statistical, systematic, and luminosity uncertainties quoted in that order.

### 10.6 Lepton asymmetries

The measurement of the charge asymmetry of the decay leptons from $W$ bosons at hadron colliders provides important information about parton distribution functions. Inclusive measurements have been performed at the Tevatron [41, 42, 43, 44], for both $W \rightarrow e v$ and $W \rightarrow \mu \nu$ events and the data have been included in global fits of parton distributions [19, 45]. The lepton asymmetry is defined as:

$$
\begin{equation*}
A=\frac{\sigma^{\varepsilon^{+}}-\sigma^{\ell^{-}}}{\sigma^{\ell^{+}}+\sigma^{\ell^{-}}} \tag{8}
\end{equation*}
$$

where in the analysis presented in this note, the fiducial cross section is used to calculate the asymmetry.
At proton-proton colliders, the overall asymmetry is predicted to be significantly different from zero as discussed in Section 3. The asymmetry varies as a function of lepton pseudorapidity since it is highly correlated with the kinematic phase space of the incoming partons and hence each $\eta$-bin probes partons with different average values of the momentum fraction.

The asymmetry $A$ is sensitive to valence quark distributions [46]. It provides complementary information to that obtained from measurements of structure functions in deep-inelastic scattering [47, $48,49,50]$, which do not strongly constrain the ratio between $u$ and $d$ quarks in the kinematic region probed at the LHC (parton momentum fraction between 0.001 and 0.1 ). In fact, the PDF parameterisations of CTEQ [37] and MSTW [19] have been shown to disagree even outside their respective errors bands [32, 51].

(a)

Figure 15: The measured values of $\sigma_{W} \cdot \mathrm{BR}(W \rightarrow \ell v)$ for $W^{+}, W^{-}$and for their sum compared to the theoretical predictions based on NNLO QCD calculations. Results are shown separately for the electron and muon channels. The predictions are shown for both proton-proton ( $W^{+}, W^{-}$and their sum) and proton-antiproton colliders $(W)$ as a function of $\sqrt{s}$. The calculations are based on the FEWZ program with the MSTW2008 NNLO structure function parameterisations (see text). In addition, measurements at previous proton-antiproton colliders are shown. The data points at the various energies are staggered to improved readability. The data points are plotted with their total uncertainty.

The $\eta$ distributions of reconstructed electrons and muons are shown to be in good agreement with the expectation (see Figure 10). The charge misidentification (the assignment of an incorrect charge to the measured lepton) is found to be negligible for muons. For electrons, it is of order of $0.1 \%$ for the barrel and $1.0 \%$ for the end-cap regions. It is implicitly taken into account in the efficiency corrections applied for the cross section.

To extract the asymmetry, QCD and $W \rightarrow \tau v$ backgrounds are subtracted from the number of observed candidates. The remaining events are corrected by the same factors as those used in the fiducial cross-section measurement. As the last step, the asymmetry is calculated for $|\eta|$ in central and end-cap bins and as well as integrated over the entire pseudorapidity range. The systematic uncertainties as discussed in the previous sections were applied to obtain the final asymmetry results. This includes the variation of the backgrounds within their associated uncertainties. However, the statistical uncertainties dominate by far the total uncertainties.

The measured lepton asymmetries as a function of $|\eta|$ are tabulated in Table 9 and shown in Figure 17. In this table, the asymmetry integrated over the full pseudorapidity range has the region $1.37<|\eta|<1.52$ excluded in both the electron and muon channels to make this number more comparable between the two channels. The statistical uncertainty on the asymmetry is determined using Gaussian error propagation from the errors on the number of observed signal events in the individual $|\eta|$ regions. If the number of events is larger than 25 , the square-root of the number of events is used for the error. If it is smaller,

(a)

Figure 16: The measured values of $\sigma_{W} \cdot \mathrm{BR}(W \rightarrow \ell v)$ for $W^{+}, W^{-}$and for their sum compared to the theoretical predictions based on NNLO QCD calculations. Results are shown for the combined electron-muon results. The predictions are shown for both proton-proton ( $W^{+}, W^{-}$and their sum) and proton-antiproton colliders $(W)$ as a function of $\sqrt{s}$. The calculations are based on the FEWZ program with the MSTW2008 NNLO structure function parameterisations (see text). In addition, measurements at previous proton-antiproton colliders are shown. The data points at the various energies are staggered to improved readability. The data points are plotted with their total uncertainty.

Poissonian confidence levels are used. These give asymmetric uncertainties on the observed number of events. As an approximation, the larger of these asymmetric uncertaintied is used in the error propagation. The asymmetry values are compared to theoretical predictions obtained with NLO calculations, namely MC@NLO [36] and DYNNLO [52] which have been interfaced to various PDF parameterisations of the respective order. The parton distribution functions MSTW08 [19], CTEQ6.6 [37] and HERAPDF 1.0 [50] were used.

## 11 Observation of $Z$ candidates

A search for $Z$ candidates was also performed in both the electron and muon channels. The preselection specifications listed in Section 6 are first applied. Subsequent requirements are made to specifically search for lepton pairs consistent with being produced from the decay of a $Z$ boson. For the electron channel, leptons pairs within $|\eta|<2.47$ are required to be of opposite charge and each lepton must pass at least the "medium" requirements as presented in Section 4.1. Events with at least one "medium" lepton in the central region of $|\eta|<2.47$ and one "forward-tight" lepton in the forward region of $2.47<|\eta|<4.9$ are also accepted. For the muon channel, the selection is loosened compared to the $W$ search: only one of the muon candidates is required to have a minimum muon combined $p_{\mathrm{T}}$ above 20 GeV . The other muon


Figure 17: Lepton charge asymmetries for the electron (a) and muon (b) channels. Superposed are several theoretical predictions (see text).

| Electron channel |  |  |  |
| :---: | :---: | :---: | :---: |
|  | $A$ | $A(\|\eta\|<1.37)$ | $A(1.52<\|\eta\|<2.47)$ |
| Measured | $0.21 \pm 0.18 \pm 0.01$ | $0.06 \pm 0.22 \pm 0.01$ | $0.54 \pm 0.40 \pm 0.01$ |
| Predicted | 0.20 | 0.16 | 0.25 |
| Muon channel |  |  |  |
|  | $A$ | $A(\|\eta\|<1.05)$ | $A(1.05<\|\eta\|<2.4)$ |
| Measured | $0.33 \pm 0.12 \pm 0.01$ | $0.32 \pm 0.18 \pm 0.01$ | $0.32 \pm 0.15 \pm 0.01$ |
| Predicted | 0.20 | 0.15 | 0.23 |

Table 9: The measured lepton asymmetries integrated over the full pseudorapidity range, as well as separately for the barrel and end-cap regions. For the electron channel: the full range represents $|\eta|<2.47$ but excludes $1.37<|\eta|<1.52$, the barrel region is $|\eta|<1.37$, and end-cap region is $1.52<|\eta|<2.47$. For the muon channel: the full range represents $|\eta|<2.4$ but excludes $1.37<|\eta|<1.52$, the barrel region is $|\eta|<1.05$, and end-cap region is $1.05<|\eta|<2.4$. The quoted uncertainties are statistical and systematic, in that order. Also quoted are the DYNNLO [52] predictions.
minimum $p_{\text {T }}$ threshold remains at 15 GeV and the pseudorapidity requirement of this second muon is relaxed to $|\eta|<2.5$. Muon candidates must have opposite charge and a muon isolation parameter $\sum p_{T}^{I D} / p_{T}<0.2$. Within the invariant mass window $m_{\ell \ell}=66-116 \mathrm{GeV}$, five candidates pass these requirements (including one candidate in the forward region) in the electron channel and nine candidates in the muon channel. Figure 18 shows the invariant masses of these candidates.

The $Z \rightarrow \ell \ell$ Monte Carlo samples discussed in Section 3 are used to estimate the number of signal events. For the electron channel, a total of $6.3 \pm 0.6$ (syst) $\pm 0.7$ (lumi) signal events with a negligible statistical uncertainty are expected for an integrated luminosity of $17.0 \mathrm{nb}^{-1}$. This estimate includes a $11 \%$ uncertainty on the luminosity and a $10 \%$ systematic uncertainty due to electron identification, energy scale, theoretical cross section uncertainty, and on the acceptance from the parton distribution functions. For the muon channel, a total of $7.9 \pm 0.8$ (syst) $\pm 0.9$ (lumi) signal events with a negligible


Figure 18: Invariant mass $m_{\ell \ell}$ of $Z$ candidates in the electron (a) and muon (b) channels. All backgrounds are too small to be shown in these figures.
statistical uncertainty are expected for an integrated luminosity of $17.7 \mathrm{nb}^{-1}$. Apart from the $11 \%$ uncertainty in luminosity determination, the primary source of systematic uncertainty in this prediction for the muon channel is the reconstruction efficiency. Since the final state in $Z \rightarrow \mu \mu$-like events contains two muons, the uncertainties in their reconstruction efficiencies are added linearly, yielding an uncertainty on the event reconstruction efficiency of $8 \%$. This number assumes that the uncertainties are fully correlated between the two muons. The uncertainty in the trigger efficiency scaling factor is $2.4 \%$. The other sources of systematic uncertainty are the same as for the $W$ channel. These contributions are added in quadrature resulting in the final number given above.

The background Monte Carlo samples in Section 3 have insufficient statistics to provide a direct estimate of the expected background events in the $Z \rightarrow e e$ channel within the mass window $66<m_{e e}<$ 116 GeV . A partially data-derived estimate is made. For the electron channel, the QCD background Monte Carlo sample may be used to estimate the number of pairs of leptons that both pass the "loose" electron requirement (either central or forward) in the appropriate mass range. A data-derived "loose" to "medium" rejection factor for the central leptons and "forward-loose" to "forward-tight" rejection factor for forward leptons are then used to estimate the expected number of lepton pairs which both pass the nominal $Z \rightarrow e e$ requirements. The ratio of "medium" to "loose" electrons with $E_{\mathrm{T}}>20 \mathrm{GeV}$, reconstructed using the standard electron algorithm of Section 4.1 and within the $\eta$ acceptance of the detector is measured in data to be $0.14 \pm 0.01$. The equivalent number for the forward region is $0.18 \pm$ 0.03 for the ratio of "forward-tight" to "forward-loose" electrons. In the $Z$ mass window $66<m_{e e}<$ 116 GeV , the Monte Carlo predicts there to be $6.9 \pm 0.7 \mathrm{QCD}$ background events in the opposite-charge invariant mass distribution for "loose" lepton pairs. By applying the data-derived rejection factors to each electron in these pairs, separating appropriately central leptons and forward leptons, a background estimate totalling $0.2 \pm 0.1$ events in the opposite-charge distribution in the $Z$ mass window is derived. The primary electroweak background directly under the mass peak $(W \rightarrow e v)$ is flat as a function of the invariant mass and expected to appear in Figure 18(a) at the $3 \times 10^{-3}$ level. $\mathrm{Z} \rightarrow \tau \tau$ background also appears at the same level but drops off sharply as a function of the invariant mass.

The total number of expected background events within the mass window $66<m_{\mu \mu}<116 \mathrm{GeV}$ in the muon channel after all requirements as estimated from Monte Carlo samples described in Table 1
is $0.04 \pm 0.01$ (syst) $\pm 0.01$ (lumi) The dominant source of background is $Z \rightarrow \tau \tau$ ( $52 \%$ ), followed by top-pair production ( $27 \%$ ). The QCD contribution ( $b \bar{b}$ events) is $17 \%$ and other sources are negligible.

## 12 Summary

This note presents a measurement by the ATLAS experiment of the $W \rightarrow \ell v$ production cross section based on $118 W \rightarrow \ell v$ candidates produced from $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions at the LHC. These results correspond to a total integrated luminosity of $16.9 \mathrm{nb}^{-1}$ for the $W \rightarrow e v$ channel, and $16.6 \mathrm{nb}^{-1}$ for the $W \rightarrow \mu \nu$ channel. The total inclusive $W$-boson production cross section times the leptonic branching ratio in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ was measured to be $(8.5 \pm 1.3($ stat $) \pm$ 0.7 (syst) $\pm 0.9$ (lumi)) nb for the $W \rightarrow e v$ channel and ( $10.3 \pm 1.3$ (stat) $\pm 0.8$ (syst) $\pm 1.1$ (lumi)) nb for the $W \rightarrow \mu \nu$ channel. This constitutes the first $W$ cross-section measurement by ATLAS in protonproton collisions and the result obtained is in agreement with theoretical calculations based on NNLO QCD. In addition the expected charge asymmetry between the cross section for $W^{+}$and $W^{-}$production is experimentally confirmed.

A total of $14 Z \rightarrow \ell \ell$ candidates was observed with an expectation of 14.2 given the integrated luminosities of $17.0 \mathrm{nb}^{-1}$ for the $Z \rightarrow e e$ channel and $17.7 \mathrm{nb}^{-1}$ for the $Z \rightarrow \mu \mu$ channel.

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ATLAS NOTE
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# Measurement of the $Z \rightarrow \ell \ell$ production cross section in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

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#### Abstract

This note describes the first measurement of the $Z \rightarrow \ell \ell$ production cross section, where $\ell=e, \mu$, by the ATLAS experiment. These results are based on $125 Z \rightarrow \ell \ell$ candidates, produced in $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions at the LHC and correspond to a total integrated luminosity of approximately $225 \mathrm{nb}^{-1}$. The total inclusive $Z$-boson production cross section times the charged leptonic branching ratio within the invariant mass window $66<m_{e e}<116 \mathrm{GeV}$ was measured to be $[0.72 \pm 0.11$ (stat) $\pm 0.10$ (syst) $\pm 0.08$ (lumi)] nb for the $Z \rightarrow e e$ channel and $[0.89 \pm 0.10$ (stat) $\pm 0.07$ (syst) $\pm 0.10$ (lumi) $] \mathrm{nb}$ for the $Z \rightarrow \mu \mu$ channel, resulting in a combined value of $[0.83 \pm 0.07$ (stat) $\pm 0.06$ (syst) $\pm 0.09$ (lumi)] nb. This constitutes the first $Z$ cross-section measurement by ATLAS in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ and the results obtained are in agreement with theoretical calculations based on NNLO QCD.


## 1 Introduction

The $W$ and $Z$ bosons are expected to be produced abundantly at the Large Hadron Collider (LHC) [1], and for the first time in proton-proton collisions. The well-known properties of the $Z$ boson will provide significant constraints in the determination of the performance of the collider experiments at the LHC; its known mass, width and leptonic decays can be exploited to determine the detector energy and momentum scale and resolution, as well as lepton identification and trigger efficiencies.

A first measurement of the $W \rightarrow \ell v$ cross section from the $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions of the LHC was presented recently [2] by the ATLAS experiment [3]. This note details a measurement of the $Z \rightarrow \ell \ell$ cross section by ATLAS. This result is based on $46 Z \rightarrow e e$ and $79 Z \rightarrow \mu \mu$ candidates resulting from a total integrated luminosity of approximately $225 \mathrm{nb}^{-1}$.

## 2 The $Z$ process and sources of background

The results presented in this note are compared to expectations based on Monte Carlo simulations. The signal and background samples used in this note were generated at $\sqrt{s}=7 \mathrm{TeV}$ with PYTHIA [4] using MRSTLO* [5] parton distribution functions (PDF), then simulated with GEANT4 [6] and fully reconstructed. Details of these samples are summarised in Table 1. For the $t \bar{t}$ samples, both MC@NLO [7, 8] and POWHEG [9] were used.

The $Z$ production cross section times its respective $Z / \gamma^{*} \rightarrow \ell \ell$ decay branching ratio used in this study is calculated to next-to-next-to-leading order (NNLO) in QCD using the FEWZ program [10] with the MSTW2008 set of parton distribution functions [11]. The invariant mass of the charged leptons from the process $Z / \gamma^{*} \rightarrow \ell \ell$ is required to be greater than 60 GeV . This value is:

$$
\begin{equation*}
\sigma_{Z / \gamma^{*} \rightarrow \ell \ell}^{N N L O}=0.99 \mathrm{nb} \tag{1}
\end{equation*}
$$

An overall uncertainty of this $Z$ cross section of $4 \%$ has been estimated using the MSTW2008NNLO PDF error eigenvectors at the $90 \%$ C.L. limit, the NNLO HERAPDF1.0 $\alpha_{s}$ variations [12], and normalisation and scale variations. In this note, the term " $Z$ cross section" will generically refer to the $Z / \gamma^{*}$ cross section.

For the electron channel, the primary backgrounds are expected to be from QCD processes, $Z \rightarrow$ $\tau \tau, W \rightarrow e v$, and $t \bar{t}$ production. These background estimates are partially derived from data and by the Monte Carlo samples described in Table 1. For the muon channel, the primary backgrounds are expected to be $Z \rightarrow \tau \tau, W \rightarrow \mu \nu, \bar{t}$, and $b \bar{b}$ production. These background estimates are derived from the Monte Carlo samples described in Table 1.

### 2.1 Event selection

The data presented in this note were collected over a four-month period, from March to July 2010. The basic beam and data-quality requirements as described in Ref. [2] resulted in total integrated luminosities of $219 \mathrm{nb}^{-1}$ for the $Z \rightarrow e e$ channel and $229 \mathrm{nb}^{-1}$ for the $Z \rightarrow \mu \mu$ channel. The uncertainty on the luminosity determination is estimated to be $11 \%$ [13].

Events are selected with the hardware-based L1 trigger as described in Ref. [2] with the following exceptions. The threshold above which the calorimeter trigger accepts electron and photon candidates increased from five to ten trigger counts, where one count corresponds to approximately 1 GeV . The muon trigger, which had no $p_{\mathrm{T}}$ threshold requirement, was changed to one whose $p_{\mathrm{T}}$ threshold is at 6 GeV , as estimated from the hit pattern of multiple chamber layers. As a result of these trigger decisions, a total of $4.4 \times 10^{6}$ and $3.8 \times 10^{6}$ events are triggered in the electron and muon channels, respectively.

| Physics process | Cross section $(\mathrm{nb})[\times \mathrm{BR}]$ | Luminosity $\left(\mathrm{nb}{ }^{-1}\right)$ |
| :--- | :---: | :---: |
| $\mathrm{Z} \rightarrow e e\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.99 | $4.8 \times 10^{6}$ |
| $\mathrm{Z} \rightarrow \mu \mu\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.99 | $5.1 \times 10^{6}$ |
| $\mathrm{Z} \rightarrow \tau \tau\left(m_{\ell \ell}>60 \mathrm{GeV}\right)$ | 0.99 | $2.0 \times 10^{6}$ |
| $\mathrm{~W} \rightarrow e \nu$ | 10.46 | $6.7 \times 10^{5}$ |
| $\mathrm{~W} \rightarrow \mu \nu$ | 10.46 | $6.7 \times 10^{5}$ |
| Dijet $\left(\right.$ electron channel, $\left.\hat{p}_{\mathrm{T}}>15 \mathrm{GeV}\right)$ | $1.15 \times 10^{6}$ | 100 |
| $b \bar{b}$ (muon channel, $\left.\hat{p}_{\mathrm{T}}>15 \mathrm{GeV}\right)$ | $7.39 \times 10^{4}$ | $59 \times 10^{3}$ |
| $c \bar{c}\left(\right.$ muon channel, $\left.\hat{p}_{\mathrm{T}}>15 \mathrm{GeV}\right)$ | $2.84 \times 10^{4}$ | $53 \times 10^{3}$ |
| $t \bar{t}($ electron channel, MC@ NLO) | 0.16 | $11 \times 10^{6}$ |
| $t \bar{t}$ (muon channel, POWHEG) | 0.16 | $2.5 \times 10^{6}$ |

Table 1: Signal and background Monte Carlo samples used in the electron and muon channel analyses, including the production cross section (multiplied by the relevant branching ratios (BR)) and the integrated luminosity of the samples. The variable $\hat{p}_{T}$ is the transverse momentum of the partons involved in the hard-scattering process. The $Z$ cross section is given at NNLO, the inclusive QCD jet and heavy quark cross sections are given at leading order (LO), and the $t \bar{t}$ cross section at NLO.

Collision candidates are selected by requiring a primary vertex with at least three tracks, consistent with the beam spot position. To reduce fake collision candidates from cosmic-ray or beam-halo events, the muon analysis requires the primary vertex position along the beam axis to be within 15 cm of the nominal position.

For the electron channel, the quality of the reconstruction of the energy deposited by the electron in the liquid argon calorimeter is assessed. The event is rejected if the candidate electromagnetic cluster is located in any problematic region of this detector [2]. These problems can cause extended dead regions in a given layer of the calorimeter, which may have an important impact on the energy reconstruction of the electron. The loss in acceptance due to this requirement is approximately $13 \%$.

## 3 Selection of $Z$ candidates

In the electron channel, pairs are formed from oppositely-charged electron-positron candidates. These lepton candidates are selected with the identification level "medium" as decribed in Ref. [2] and are required to have a cluster transverse energy $E_{\mathrm{T}}>20 \mathrm{GeV}$ within the pseudorapidity range $|\eta|<2.47$, excluding the transition region between the barrel and end-cap calorimeters ( $1.37<|\eta|<1.52$ ).

In the muon channel, pairs are formed from oppositely-charged muon candidates. These lepton candidates are required to be combined muons (stand-alone muon spectrometer tracks associated to an inner-detector (ID) tracks) with transverse momentum $p_{\mathrm{T}}>20 \mathrm{GeV}$ as well as have their $p_{\mathrm{T}}$ as measured by the muon spectrometer greater than 10 GeV , within the range $|\eta|<2.4$. The difference between the inner-detector and muon-spectrometer $p_{\mathrm{T}}$, corrected for the mean energy loss in upstream material, is required to be less than 15 GeV to increase the robustness against track reconstruction mismatches. All muon candidates must satisfy the muon isolation parameter requirement $\sum p_{T}^{I D} / p_{T}<0.2$ in a narrow cone of size 0.4 in pseudorapidity-azimuthal angle space. The minimum $-p_{\mathrm{T}}$ used in the isolation requirement is 1 GeV . The difference between the $z$ position of the muon spectrometer tracks extrapolated to the beam line and the $z$ coordinate of the primary vertex is required to be less than 1 cm .

Table 2 summarises the number of $Z \rightarrow \ell \ell$ candidates remaining in data after all requirements have been imposed. A total of 46 candidates pass all requirements in the electron channel and 79 candidates in the muon channel within the invariant mass window $m_{\ell \ell}=66-116 \mathrm{GeV}$. Figure 1 shows the electron

|  | Electron channel | Muon channel |
| :--- | :---: | :---: |
| Requirement | Number of <br> candidates | Number of <br> candidates |
| Triggered | $4.4 \times 10^{6}$ | $3.8 \times 10^{6}$ |
| $\ell^{+} \ell^{-}$pairs | 51 | 85 |
| $66<m_{\ell^{+}+\ell^{-}}<116 \mathrm{GeV}$ | 46 | 79 |

Table 2: Number of $Z \rightarrow \ell \ell$ candidates in data.


Figure 1: Electron cluster $E_{\mathrm{T}}(a)$ and muon $p_{\mathrm{T}}$ (b) of the $Z$ candidate leptons after final selection.
cluster $E_{\mathrm{T}}$ and muon combined $p_{\mathrm{T}}$ of the lepton candidates. The breakdown of the various background contributions are also shown in this figure. Only the electroweak and $\bar{t}$ backgrounds are shown in the electron channel due to the lack QCD Monte-Carlo samples with sufficient statistics. Instead, this component will be measured from the data, as described in Section 4. Due to the small size of the backgrounds in both the electron and muon channels, backgrounds are not shown in subsequent plots. Figure 2 shows the $p_{\mathrm{T}}$ spectrum of the $Z \rightarrow \ell \ell$ candidates. It is to be noted that all data distributions in this note are given with statistical error bars only, corresponding to $68.3 \%$ confidence intervals unless otherwise specified and that the Monte-Carlo distributions are normalised to the total luminosity.

The invariant mass distribution of these opposite-charged candidate leptons is presented in Figure 3. In Figure 4, a fit is superposed to these data. The data are modelled using the theoretical lineshape, including photon and $Z$ contributions, convolved with a gaussian resolution function. The fitted peak of the distribution is found to be $[88.7 \pm 0.8$ (stat) $] \mathrm{GeV}$ in the electron channel, and $[89.3 \pm 0.8$ (stat) $] \mathrm{GeV}$ in the muon channel (with values of 90.6 GeV and 91.2 GeV , respectively, from the Monte Carlo). The experimental resolution is found to be $[3.6 \pm 0.8$ (stat) $] \mathrm{GeV}$ and $[4.2 \pm 0.8$ (stat) $] \mathrm{GeV}$ (with values of 1.7 GeV and 1.8 GeV from the Monte Carlo), respectively. These results are within the electromagnetic calorimeter expected energy scale and resolution based on test-beam measurements and first in-situ measurements of $\pi^{0} \rightarrow \gamma \gamma$ [14]. The increase of the $Z$ width in the muon channel is due mostly to inner-detector alignment modes affecting high $-p_{\mathrm{T}}$ tracks and misalignments in the forward region of the muon spectrometer.


Figure 2: $p_{\mathrm{T}}$ of the $Z$ candidates in the electron channel (a) and muon channel (b) after final selection.

## 4 Background expectations for the $Z \rightarrow \ell \ell$ candidates

A partially data-derived estimate of the QCD background is made for the electron channel using the same procedure as described in Ref [2] and using the same QCD scale factor as observed in that measurement. A QCD background Monte Carlo sample is used to estimate the number of pairs of charged leptons that both pass the "loose" electron requirement ( as decribed in Ref. [2]) within the mass window $66<m_{e e}<$ 116 GeV . A data-derived "loose" to "medium" rejection factor for the leptons is then used to estimate the expected number of lepton pairs which both pass the nominal $Z \rightarrow e e$ requirements. The ratio of "medium" to "loose" electrons with $E_{\mathrm{T}}>20 \mathrm{GeV}$ within the $\eta$ acceptance of the detector is measured in data to be $0.15 \pm 0.01$ (stat). This result is consistent with the equivalent number derived from the QCD background Monte Carlo. In the $Z$ mass window $66<m_{e e}<116 \mathrm{GeV}$, the Monte Carlo predicts $14.2 \pm 3.4$ (stat) QCD background events in the opposite-charge invariant mass distribution for "loose" lepton pairs. By applying the data-derived rejection factors to each electron in these pairs, a background estimate totalling $0.31 \pm 0.07$ (stat) $\pm 0.05$ (syst) events in the opposite-charge distribution in the $Z$ mass window is derived. Within the mass window $66<m_{e e}<116 \mathrm{GeV}$, the remaining sources of backgrounds ( $W \rightarrow e v: 0.06$ events and $\bar{t}: 0.08$ events) are expected to be flat as a function of the invariant mass while $\mathrm{Z} \rightarrow \tau \tau$ background ( 0.04 events) is expected to drop off sharply. The total expected background within the invariant mass window $66<m_{e e}<116 \mathrm{GeV}$ is then $0.49 \pm 0.07$ (stat) $\pm 0.05$ (syst) events.

The total number of expected background events in the muon channel within the mass window $66<$ $m_{\mu \mu}<116 \mathrm{GeV}$ after all requirements as estimated from Monte Carlo samples described in Table 1 is $0.17 \pm 0.01$ (stat) $\pm 0.01$ (syst) and consists of $\bar{t}$ ( 0.08 events), $Z \rightarrow \tau \tau$ ( 0.06 events), $b \bar{b}$ ( 0.02 events), and $W \rightarrow \mu \nu$ ( 0.01 events). All other sources of background are negligible in comparison.

The number of same-charge lepton pairs that otherwise satisfy all other requirements is a good indicator of the level of background in the selection. In the electron channel, only one same-charge lepton pair (at $m_{e e}=82.8 \mathrm{GeV}$ ) satisfies all $Z$ selection requirements within the invariant mass window while there are none in the muon channel.


Figure 3: Invariant mass $m_{\ell \ell}$ of $Z$ candidates in the electron (a) and muon $(b)$ channels.

## 5 Cross-section measurements for Z-boson decays to electrons and muons

### 5.1 Introduction

The Z-boson cross-section measurement is given by:

$$
\begin{equation*}
\sigma_{t o t}=\sigma_{Z / \gamma^{*}} \times B R\left(Z / \gamma^{*} \rightarrow \ell \ell\right)=\frac{N_{Z}^{s i g}}{A_{Z} C_{Z} L_{i n t}} \tag{2}
\end{equation*}
$$

where $\sigma_{\text {tot }}$ is measured within the invariant mass window $m_{\ell \ell}=66-116 \mathrm{GeV}$ and

- $N_{Z}^{s i g}$ denotes the number of background-subtracted signal events in the channel of interest, as summarised in Table 4;
- $A_{Z}$ denotes the so-called geometrical acceptance for the $Z$-boson decays under consideration, defined as the fraction of decays satisfying the geometrical and kinematical (fiducial) constraints at the generator level. These include the $\eta$ requirements as given in Section 3, as well as requirements on $p_{\mathrm{T}}{ }^{\ell}>20 \mathrm{GeV}$ for the electron and muon channels. These acceptance values are calculated within the invariant mass window $m_{\ell \ell}=66-116 \mathrm{GeV}$ and can only be determined from $Z \rightarrow \ell \ell$ Monte Carlo simulation at generator level;
- $C_{Z}$ denotes the ratio between number of signal events which pass the final selection requirements after reconstruction and the total number of generated events within the geometrical acceptance. In this note, $C_{Z}$ is estimated using Monte Carlo signal simulation, but this correction factor includes the efficiency for triggering on lepton candidates as well as reconstructing/identifying $Z$-boson decays falling within the geometrical acceptance. In this note, the correction factors $C_{Z}$ are taken from simulation for the electron channel, but some data-derived corrections are used for the muon channel, as described in Section 5.3. The effect of final state radiation (QED) and event migration from outside the mass window, evaluated with the full simulation of the detector, is also absorbed into this factor;
- and $L_{i n t}$ denotes the integrated luminosity for the channel of interest.


Figure 4: Invariant mass $m_{\ell \ell}$ of $Z$ candidates in the electron $(a)$ and muon $(b)$ channels. The data are modelled using the theoretical lineshape, including photon and $Z$ contributions, convolved with a gaussian resolution function.

The geometrical acceptance $A_{Z}$, as well as the denominator of $C_{Z}$, are computed at the Born level, i.e. from lepton kinematics before QED corrections. The factor $C_{Z}$ thus includes the corrections for the final state radiation.

Equation 2 defines the measured total inclusive cross sections for each channel, $\sigma_{t o t}$, measured within the invariant mass window $m_{\ell \ell}=66-116 \mathrm{GeV}$ and. Equation 2 with the geometrical acceptance $A_{Z}$ set to unity defines the measured fiducial inclusive cross sections $\sigma_{\text {fid }}$ for each channel. These fiducial cross sections do not rely strongly on any theoretical prediction for the geometrical acceptance and therefore do not contain significant theoretical uncertainties related to it. Cross-section results in this note will be presented for both the electron and muon channels.

### 5.2 Electron efficiencies and systematic uncertainty on $C_{Z}$

The correction factor $C_{Z}$ includes as a primary component the efficiency for reconstructing and identifying $Z$-boson decays falling within the geometrical acceptance. An important efficiency component for the electron channel is the "medium" electron reconstruction/identification efficiency measured with respect to all reconstructed electron candidates. Its average value is 0.863 . A total systematic uncertainty of $\pm 11 \%$ is assigned to the "medium" electron identification efficiency and comes from material interaction effects upstream of the calorimeter, the impact of event pile-up in the detector, as well as observed discrepancies in the electron identification variables, as mentioned below. This "medium" electron identification efficiency is calculated with respect to all reconstructed candidate electrons and so additional factors must be taken into account for electrons that are in the acceptance but, due to various effects, fail to be reconstructed as candidate electrons. Important sources of loss of approximately $17 \%$ are due to problematic regions of the calorimeter as specified in Section 2.1 as well as kinematic and $E_{\mathrm{T}}$ requirements. Other sources of loss are due to the mass window and opposite-charge requirements. The correction factor $C_{Z}$ in addition accounts for the very small inefficiencies for selecting collisions with a reconstructed primary vertex and also includes contributions from trigger effects. The total systematic uncertainty on $C_{Z}$ is then the sum in quadrature of the following contributions:

- Trigger efficiency: The trigger efficiency has been measured in data to be $(99.8 \pm 0.2) \%$;
- Discrepancies in electron identification variables: Some discrepancies in electron identification variables have been observed for both electron and photon candidates. A systematic uncertainty was obtained by shifting the observed shapes for the Monte Carlo signal electrons from Z-boson decay to match those observed for electron candidates in the same kinematic range in data. A systematic uncertainty of $\pm 10 \%$ is assigned to $C_{Z}$;
- Pile-up: The impact of pile-up on the "medium" electron identification efficiency is evaluated with dedicated pile-up Monte-Carlo samples. A total systematic uncertainty of $\pm 2 \%$ is assigned to $C_{Z}$;
- Material effects: The impact of possible extra material in the inner detector and in front of the active EM calorimeter has been evaluated with a dedicated simulation as described in Ref. [2]. There are two components that contribute to the overall systematic uncertainty due to this effect: impact on the reconstruction of candidate electrons and on the "medium" electron identification efficiency. A total systematic uncertainty of $\pm 8 \%$ is assigned to $C_{Z}$;
- Problematic regions in the calorimeter: An additional uncertainty is attributed to electrons that fail to be reconstructed due to problematic regions in the liquid argon calorimeter. A total systematic uncertainty of $\pm 4 \%$ is assigned to $C_{Z}$;
- Energy scale and resolution: The impact of the electron scale and resolution is dominated by the estimated uncertainty on the EM calorimeter energy scale of $\pm 3 \%$ based on test-beam measurements and first in-situ measurements of $\pi^{0} \rightarrow \gamma \gamma$ [14]. Varying the energy scale by this factor provides an uncertainty of $\pm 2 \%$ on $C_{Z}$.

In summary, the final correction $C_{Z}$ is 0.645 with a total systematic uncertainty of $\pm 14 \%$.

### 5.3 Muon efficiencies, scale factors, and uncertainty on $C_{Z}$

Several important components such as muon reconstruction and trigger efficiencies feed into the evaluation of $C_{Z}$ and its systematic uncertainty. These efficiencies have been determined in Monte Carlo and corrected by data-driven scale factors to take into account differences between data and simulation. The muon reconstruction efficiency as determined from the Monte Carlo and corrected by the scale factor is $0.98 \pm 0.01$ (stat) $\pm 0.03$ (syst). This scale factor of $1.00 \pm 0.01$ (stat) $\pm 0.03$ (syst) was obtained from efficiency studies of isolated combined muon tracks relative to inner detector tracks matched to muon hits in the muon spectrometer which reduce the contribution of fake muons. The inner-detector track efficiency and the muon hit efficiency are considered well modelled in the Monte Carlo, and a systematic is assigned to the level of agreement of this assumption.

The trigger efficiency of $0.84 \pm 0.01$ (stat) $\pm 0.02$ (syst) was obtained by correcting the value obtained in Monte Carlo with the correction factors $0.98 \pm 0.01$ (stat) $\pm 0.02$ (syst) measured from data. These results have been derived by comparing the relative trigger efficiency for reconstructed muons above 15 GeV in data and simulations for both barrel and end-cap trigger systems.

The systematic uncertainty on $C_{Z}$ comes in part from the uncertainties on the reconstruction and trigger efficiencies mentioned above. Other effects are due to inefficiencies for selecting collisions with a reconstructed primary vertex, as well as the muon scale and resolutions. The total systematic uncertainty on $C_{Z}$ is then the sum in quadrature of the following contributions:

- Muon reconstruction: This systematic uncertainty of $\pm 7 \%$ is dominated by the dependence of the efficiency on the transverse momenta and the uncertainty on the remaining $\pi / \mathrm{K}$ contamination in the data sample where the efficiency is measured;

| MC | $A_{Z}$ | $A_{Z}$ |
| :--- | :--- | :--- |
|  | $Z \rightarrow e e$ | $Z \rightarrow \mu \mu$ |
| PYTHIA MRSTLO* | 0.446 | 0.486 |
| MC@NLO HERAPDF1.0 | 0.440 | 0.479 |
| MC@NLO CTEQ6.6 | 0.445 | 0.485 |

Table 3: Summary of geometrical acceptance values $A_{Z}$ for $Z \rightarrow e e$ and $Z \rightarrow \mu \mu$ using various MonteCarlo simulations.

- Trigger efficiency: This uncertainty of $\pm 2 \%$ is derived by changing the tolerance on the matching between tracks and trigger signals and comparing measurements obtained in different trigger data streams. This number is a weighted average of the barrel and end-cap trigger efficiency uncertainties, taking into account that there are two muons that can pass the trigger requriements;
- Energy scale and resolution: This uncertainty estimation is obtained by applying a smearing of Monte Carlo muon momentum resolution and scale using parameters in agreement with the data (energy scale uncertainty of $2 \%$ and a resolution uncertainty of $5 \%$ in the barrel and $8.5 \%$ in the end-cap [15]) A systematic uncertainty of $\pm 1 \%$ is assigned to $C_{Z}$.

The final $C_{Z}$ is 0.797 with a total systematic uncertainty of $\pm 7 \%$.

### 5.4 Geometrical acceptance and uncertainty

The calculation of the total cross section takes into account the phase-space requirements applied in the fiducial cross-section measurement and is entirely based on Monte-Carlo simulations. This geometrical acceptance factor, $A_{Z}$, is defined as

$$
\begin{equation*}
A_{Z}=\left(\frac{N^{a c c}}{N^{\text {all }}}\right)_{\text {gen }}, \tag{3}
\end{equation*}
$$

where $N^{a c c}$ is the number of generated events that pass the fiducial requirements (accepted events as defined in Section 3) and $N^{\text {all }}$ is the total number of generated events (both values are calculated within the mass window $66<m_{\ell \ell}<116 \mathrm{GeV}$ ). The effect of event migration from below and above the mass window is taken into account in $C_{Z}$, which has been evaluated using events generated with $\sqrt{\hat{s}}>60 \mathrm{GeV}$. The quantity $A_{Z}$ is determined before the final-state radiation and the losses due to this effect become a component of the $C_{Z}$, evaluated with the full simulation of the detector response [16].

The acceptance is calculated using the PYTHIA $Z$ samples generated with the modified LO parton distribution function (PDF) MRSTLO* [5] and the corresponding ATLAS MC09 tune [17]. The central values of the acceptances are provided in Table 3. The statistical uncertainty resulting from the Monte Carlo sample is negligible.

The systematic uncertainties on the acceptance are dominated by the limited knowledge of the proton PDFs and the modelling of the Z-production at the LHC. These uncertainties are evaluated using dedicated MC@NLO [18] samples generated with two different NLO PDFs: the CTEQ6.6 PDF [19] and HERAPDF1.0 [20]. The acceptance results determined with these alternate PDFs are presented in Table 3.

The systematic uncertainty on the acceptance is derived from the following sources:

- The difference for the MC@NLO acceptances using the two PDFs is $1.3 \%$;
- The uncertainty due to the CTEQ6.6 PDF error eigenvector sets on $A_{Z}$ is evaluated using a PDF reweighting technique and is estimated to be $\pm 1.6 \%$;
- The MC@NLO HERAPDF1.0 acceptance values are smaller than PYTHIA values by $1.5 \%$.

|  | Z |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Electron channel |  |  |  | Muon channel |  |  |  |
|  | value | stat | syst | lumi | value | stat | syst | lumi |
| Background- <br> subtracted signal | 45.5 | 6.8 | - | - | 78.8 | 8.9 | - | - |
| Correction $C_{Z}$ | 0.645 | - | 0.090 | - | 0.797 | 0.013 | 0.053 | - |
| Fiducial cross section (nb) | 0.32 | 0.05 | 0.05 | 0.04 | 0.43 | 0.05 | 0.03 | 0.05 |
| Acceptance $A_{Z}$ | 0.446 | - | 0.013 | - | 0.486 | - | 0.014 | - |
| Total cross section (nb) | 0.72 | 0.11 | 0.10 | 0.08 | 0.89 | 0.10 | 0.07 | 0.10 |

Table 4: Results for the fiducial cross sections $\sigma_{\text {fid }}$ and total cross section $\sigma_{\text {tot }}$ for $Z$ in the electron and muon channels. Shown are the observed numbers of signal events after background subtraction for each channel, the average correction factors $C_{Z}$, the fiducial cross sections, the geometrical acceptance correction factors, and the total cross sections with their statistical, systematic, and luminosity uncertainties quoted in that order.

These components added in quadrature result in systematic uncertainties on the acceptance values of $2.5 \%$. Due to the limited choice of samples and knowledge about correlations between the contributions, the acceptance-related uncertainty on the $Z$ cross-section measurement is taken to be $3 \%$, motivated by studies from Ref. [2].

### 5.5 Measured cross sections

All of the elements necessary to calculate the fiducial and total cross sections for $Z$ production and decay in the electron and muon channels are summarised in Table 4. The background-subtracted number of signal events consists of the 46 (79) observed candidates events in the electron (muon) channel as given in Table 2 minus the 0.49 ( 0.17 ) background events in the electron (muon) channel as described in Section 4.

The derived fiducial and total cross sections for both the electron and muon channels within the invariant mass window $66<m_{e e}<116 \mathrm{GeV}$ are also presented in this table, along with their statistical , systematic, and luminosity uncertainties. The total cross section value for the combined electronmuon channels, when taking into account the correlated and uncorrelated sources of uncertainty, is $\sigma_{\text {tot }}=[0.83 \pm 0.07$ (stat) $\pm 0.06$ (syst) $\pm 0.09$ (lumi) $] \mathrm{nb}$.

### 5.6 Comparison to theoretical calculations

A comparison of the measured cross-section value to theoretical predictions including next-to-next-to-leading order QCD corrections is shown in Figure 5 (where the electron and muon channels are shown separately) and Figure 6 (where the electron and muon channels are combined). The calculations were performed with the program FEWZ [10] using the MSTW2008 NNLO parton density function parameterisation [11]. The renormalisation scale $\mu_{R}$ and factorisation scale $\mu_{F}$ were chosen to be $\mu_{F}=\mu_{R}=m_{Z}$. Within the experimental uncertainties, the measured cross section agrees well with the calculation $\sigma_{\text {tot }}=(0.964 \pm 0.039) \mathrm{nb}$ within the invariant mass window $66<m_{e e}<116 \mathrm{GeV}$. It should be noted that the theoretical uncertainties resulting from variations of the renormalisation and factorisation scales as well as uncertainties resulting from parton density function parameterisations are not shown in these figures. As discussed in Section 2, these uncertainties are expected to be of the order of $\pm 4 \%$ at 7 TeV . Figures 5 and 6 also display the results of previous measurements of the total $Z$ production

(a)

Figure 5: The measured value of $\sigma_{Z / \gamma^{*}} \times \mathrm{BR}\left(Z / \gamma^{*} \rightarrow \ell \ell\right)$ presented for the electron and muon channels separately, compared to the theoretical predictions based on NNLO QCD calculations. The predictions are shown for both proton-proton and proton-antiproton colliders as a function of $\sqrt{s}$. The calculations are based on the FEWZ program with the MSTW2008 NNLO parton density function parameterisations (see text). In addition, measurements at previous proton-antiproton colliders are shown. The data points at the various energies are staggered to improve readability. The data points are plotted with their total uncertainty.
cross section by the CDF [21] and D0 [22] experiments at $\sqrt{s}=1.96 \mathrm{TeV}$ at the Fermilab Tevatron collider and by the UA1 [23] and UA2 [24] experiments at $\sqrt{s}=0.63 \mathrm{TeV}$ at the CERN Sp $\overline{\mathrm{p} S}$ protonantiproton collider. All measurements are in good agreement with the theoretical prediction. The energy dependence of the total $Z$-production cross section is well described.

## 6 Summary

This note presents a measurement by the ATLAS experiment of the $Z \rightarrow \ell \ell$ production cross section based on 125 candidates produced from $\sqrt{s}=7 \mathrm{TeV}$ proton-proton collisions at the LHC. These results correspond to a total integrated luminosity of approximately $225 \mathrm{nb}^{-1}$. The total inclusive Z-boson production cross section times the charged leptonic branching ratio in proton-proton collisions at $\sqrt{s}=$ 7 TeV was measured to be $[0.72 \pm 0.11$ (stat) $\pm 0.10$ (syst) $\pm 0.08$ (lumi) $] \mathrm{nb}$ for the $Z \rightarrow e e$ channel and $[0.89 \pm 0.10$ (stat) $\pm 0.07$ (syst) $\pm 0.10$ (lumi) $] \mathrm{nb}$ for the $Z \rightarrow \mu \mu$ channel, resulting in a combined result of $[0.83 \pm 0.07$ (stat) $\pm 0.06$ (syst) $\pm 0.09$ (lumi) $] \mathrm{nb}$ all measured within the invariant mass window $66<m_{e e}<116 \mathrm{GeV}$. This constitutes the first $Z$ cross-section measurement by ATLAS in proton-proton collisions and the result obtained is in agreement with theoretical calculations based on NNLO QCD.

(a)

Figure 6: The measured value of $\sigma_{Z / \gamma^{*}} \times \mathrm{BR}\left(Z / \gamma^{*} \rightarrow \ell \ell\right)$ where the electron and muon channels have been combined, compared to the theoretical predictions based on NNLO QCD calculations. The predictions are shown for both proton-proton and proton-antiproton colliders as a function of $\sqrt{s}$. The calculations are based on the FEWZ program with the MSTW2008 NNLO parton density function parameterisations (see text). In addition, measurements at previous proton-antiproton colliders are shown. The data points at the various energies are staggered to improve readability. The data points are plotted with their total uncertainty.

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ATLAS NOTE
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# Evidence for prompt photon production in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

The ATLAS Collaboration


#### Abstract

Photon identification is important for many physics signatures at the LHC. Prompt photon identification in ATLAS relies on the fine granularity of the electromagnetic calorimeter, which provides event-by-event rejection of the dominant background from photons produced by $\pi^{0}$ decays, and on the inner detector, which allows the reconstruction of photon conversions to electron-positron pairs. This note describes the extraction of the isolated prompt photon signal above the background for data from $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$, corresponding to an integrated luminosity of $15.8 \mathrm{nb}^{-1}$, collected with the ATLAS detector at the LHC. Using a two-dimensional sideband background subtraction technique, a statistically significant signal of prompt photons is observed, with a yield $N=(618 \pm 72)$ and a purity $P=(72 \pm 7) \%$ for transverse energies above 20 GeV .


## 1 Introduction

Prompt photon production at hadron colliders provides a handle for testing perturbative QCD predictions [1]. It can also be used to constrain parton structure functions [2]. Furthermore, photon identification is important for many physics signatures, including searches for Higgs boson or graviton decays to photon pairs, decays of excited fermions, and decays of pairs of supersymmetric particles, characterized by the production of two energetic photons and large missing transverse energy. As the Standard Model cross section for inclusive prompt photon production at LHC energies is expected to be rather large, $O(\mu \mathrm{~b})$ for transverse energies above $10 \mathrm{GeV}[3,4]$, a search of this process can already be performed in ATLAS with a modest integrated luminosity. Recent measurements of the inclusive prompt photon production cross section at the Tevatron, in $p \bar{p}$ collision at a centre-of-mass energy $\sqrt{s}=1.96 \mathrm{TeV}$, are reported in Refs. [5, 6].

In the following, all photons produced in proton-proton collisions not coming from hadron decays are considered as "prompt". In Monte-Carlo computation, these include the photons that are either:

- originating from hard-scattering processes,
- emitted from QED radiation off quarks in the initial or final state, or
- produced from non-perturbative fragmentation of quarks and gluons.


Figure 1: Inclusive prompt photon production cross section expected from QCD using the next-to-leading order (NLO) JETPHOX computation, for photons with pseudorapidity $|\eta|<1.37$ or $1.52<|\eta|<2.37$ and transverse energies above 10 GeV .

As an example, Figure 1 shows the expected differential cross section from the NLO QCD computation implemented in the JETPHOX program [3], for prompt photons with transverse energies $\left(E_{\mathrm{T}}\right)$ above 10 GeV and within the pseudorapidity $(\eta)$ acceptance of the ATLAS photon identification. A parton level isolation cut, requiring a total transverse energy below 5 GeV from the partons inside a cone of radius
$\Delta R=\sqrt{\Delta \eta^{2}+\Delta \phi^{2}}=0.4$ in $\eta \times \phi$ around the photon direction, has been used for this computation. This is expected to be close to the experimental isolation cut applied to the data. Varying the parton level isolation cut from 5 to 3 GeV changes the predicted cross section by $3 \%$. Figure 1 also shows the expected factorization and renormalization scale uncertainty (varied between 0.5 and 2.0 times the nominal scale which was set to the transverse energy of the photon) and the expected structure function uncertainty using CTEQ6.1 [7].

In a hadron collider environment, the main background is composed by photons from decays of light neutral mesons like $\pi^{0}$ or $\eta$. They will be called "fake" photons in the following. This note describes how a signal of isolated prompt photons with transverse energies above 10 GeV can be extracted from the background in the early ATLAS data. In Section 2, the note begins by briefly recalling the main characteristics of the ATLAS detector. Section 3 summarizes the data and simulated samples used for this analysis. Section 4 describes the various steps of the photon identification together with a comparison between data and Monte Carlo (MC) simulations. Section 5 illustrates the expected photon identification and trigger efficiencies. Section 6 describes the methods used to derive from the data the background level and to extract the prompt photon signal, together with the associated systematic uncertainties.

## 2 The ATLAS detector

The ATLAS detector is described in detail in Ref. [8]. We summarize here the main features of the subdetectors which are more relevant to this analysis: the calorimeter, in particular its electromagnetic section, and the inner detector.

The electromagnetic calorimeter is a lead-liquid Argon (Pb-LAr) sampling calorimeter with accordion geometry. It is divided in a barrel section covering the pseudorapidity region $|\eta|<1.45$ and two end-cap sections covering the pseudorapidity regions $1.375<|\eta|<3.2$. It consists of three longitudinal layers. The first one, with a thickness between 3 and 5 radiation lengths, has a very high granularity in the $\eta$ direction (between 0.003 and 0.006 depending on $\eta$, with the exception of the regions $1.4<|\eta|<1.5$ and $|\eta|>2.4$ ), sufficient to provide an event-by-event discrimination between single photon showers and double nearby showers coming from a $\pi^{0}$ decay. The second layer of the electromagnetic calorimeter, which collects most of the energy deposited in the calorimeter by the photon shower, has a thickness around 17 radiation lengths and a granularity of $0.025 \times 0.025$ in $\eta \times \phi$, where $\phi$ is the azimuthal coordinate around the beam $z$ axis. A third layer, with thickness varying between 4 and 15 radiation lengths, is used to correct leakage beyond the calorimeter for high energy showers. Before the accordion calorimeter, a thin presampler layer, covering the pseudorapidity interval $|\eta|<1.8$, is used to correct fluctuations of energy loss before the calorimeter. The sampling term $a$ of the energy resolution $(\sigma(E) / E \approx a / \sqrt{E(\mathrm{GeV})})$ varies between $10 \%$ and $17 \%$ as a function of $|\eta|$ [9] and it is the largest contribution to the resolution up to about 200 GeV , where the global constant term $(0.7 \%)$ starts to dominate [10]. During the April and May 2010 data taking, about 20 out of 1524 optical links of the calorimeter readout system were non working, in addition approximately $0.05 \%$ of single channels were affected by readout problem or noise and masked during reconstruction.

A hadronic sampling calorimeter is located beyond the electromagnetic calorimeter. It is made of steel and scintillating tiles in the barrel section, with depth around 7.4 interaction lengths, and of two wheels of copper and liquid argon in each end-cap, with depth around 9 interaction lengths. In this analysis the hadronic calorimeter is used to reduce background due to photons from neutral hadron decays, exploiting the fact that energy leakage in the hadronic calorimeters from isolated prompt photons is much lower than that for fake photons from decays of $\pi^{0}$ or other neutral hadrons in jets, since the latter are accompanied by nearby hadrons produced in the same jet.

The inner detector is comprised of three subsystems: at small radial distance $R$ from the beam axis ( $50.5<R<150 \mathrm{~mm}$ ), pixel silicon detectors are arranged in three cylindrical layers in the barrel and
in three disks in each end-cap; at intermediate radii ( $299<R<560 \mathrm{~mm}$ ), double layers of single-sided silicon microstrip detectors are used, organized in four cylindrical layers in the barrel and nine disks in each end-cap; at larger radii ( $563<R<1066 \mathrm{~mm}$ ), a straw tracker with transition radiation capabilities divided into one barrel section (with 73 layers of straws parallel to the beam line) and two end-caps (with 160 layers each of straws radial to the beam line) is used. These three systems are immersed in a 2 T axial magnetic field provided by a superconducting solenoid. The inner detector has full coverage in $\phi$. The silicon pixel and strip subsystems cover the pseudorapidity range $|\eta|<2.5$, while the transition radiation tracker acceptance is limited to the range $|\eta|<2.0$. The inner detector allows an accurate reconstruction of tracks from the primary proton-proton collision point and also from secondary vertices, permitting an efficient reconstruction of photon conversions in the inner detector material up to a radius of $\approx 80 \mathrm{~cm}$.

The total amount of material before the first active layer of the electromagnetic calorimeter (including the presampler) varies between 2.5 and 6 radiation lengths as a function of pseudorapidity, excluding the transition region $(1.37<|\eta|<1.52)$ between the barrel and the end-caps, where the material thickness increases to 11.5 radiation lengths. A proper description of this material is important for accurate modeling of the calorimeter response including the detailed shape of electromagnetic showers.

## 3 Data sample

This analysis is based on proton-proton collision data collected at a centre-of-mass energy $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector at the LHC in April and May 2010. Events are triggered using the first level (L1) calorimeter trigger, based on the energy deposits in the electromagnetic calorimeter. Using a rougher granularity $(0.1 \times 0.1$ in $\eta \times \phi)$ than that of the electromagnetic calorimeter, electromagnetic clusters with fixed size $0.2 \times 0.2$ are searched for and retained if the total transverse energy in two of their four trigger channels is above a certain programmable threshold. The trigger used in this analysis uses a threshold of 5 GeV , which reaches a plateau of constant efficiency close to $100 \%$ for true photons with $E_{\mathrm{T}}>10$ GeV . Given the moderate peak luminosity $\left(\approx 2 \times 10^{29} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}\right)$, the trigger can be operated at a tolerable rate $(\leq 30 \mathrm{~Hz})$ without prescaling, so that no higher level trigger selection is required. The calorimeter and inner detector are required to be fully operational with good data quality. The collected sample corresponds to an integrated luminosity of $15.8 \pm 1.7 \mathrm{nb}^{-1}$.

For this analysis, events are required to have a reconstructed primary vertex consistent with the average beam spot position and with at least three associated tracks. The efficiency of this requirement is $99.5 \%$ in the data sample and is expected to be around $99.9 \%$ for events containing prompt photons with transverse energies above 10 GeV . The distribution of the time difference between the signals observed in the two endcaps of the detector shows that non-collision background is negligible. The total number of selected events is 2.27 million.

To study the characteristics of signal and background events, Monte Carlo samples are generated using the PYTHIA event generator [11], with parameters set according to the ATLAS MC09 tune [12], and the ATLAS detector response is simulated using the GEANT4 program [13]. These samples are then reconstructed with the same algorithms used for data. More details on the event generation and simulation infrastructure of the ATLAS experiment are provided in Ref. [14]. For the signal, a sample of hard-scattering photons (hard subprocesses $q g \rightarrow q \gamma$ and $q \bar{q} \rightarrow g \gamma$ ) with generated transverse momenta above 7 GeV is used. The equivalent luminosity of this sample, computed assuming a cross section of $1.4 \mu \mathrm{~b}$ as obtained from PYTHIA, is $71 \mathrm{nb}^{-1}$. To study background processes, two samples are simulated. In the first one, generated non-diffractive minimum bias events are filtered requiring at least 6 GeV of transverse energy in a $0.18 \times 0.18$ region in $\eta \times \phi$ at the truth particle level, mimicking a calorimetric L1 trigger requirement. The events passing this filter, whose efficiency is around $5.3 \%$, are then fully simulated. This filter is found to be unbiased for transverse energies above 10 GeV . The equivalent integrated luminosity of this sample, according to the effective production cross section (including the
filter efficiency) $\sigma=2.58 \mathrm{mb}$ returned by PYTHIA, is $11.6 \mathrm{nb}^{-1}$. Since the $E_{\mathrm{T}}$ spectrum of reconstructed fake candidates decreases rapidly above the filter threshold, a second sample, enriched in candidates with higher transverse energies, is used to study fake photon candidates with reconstructed $E_{T}>20 \mathrm{GeV}$. In this sample all relevant $2 \rightarrow 2$ QCD hard subprocesses are switched on, the transverse momentum of the hard-scattering products is required to be greater than 15 GeV and the same filter as for the minimum bias sample, but with a higher threshold at 17 GeV , is used before the full simulation. This sample is found to be unbiased for transverse energies above 20 GeV . Its equivalent integrated luminosity, according to the effective production cross section $\sigma=0.99 \mathrm{mb}$ computed with PYTHIA (taking into account also the filter efficiency, $8.6 \%$ ), is $101 \mathrm{nb}^{-1}$. These QCD background samples contain "fake" photon candidates, as well as prompt photon signals produced by QED radiation emitted from quarks. The higher energy sample contains also the contribution of prompt gamma-jet hard-scattering contribution. Prompt photon contributions are removed when studying background contribution with these samples.

## 4 Photon identification and isolation

Photon reconstruction and identification is seeded by energy clusters in the electromagnetic calorimeter with transverse energies exceeding 2.5 GeV in projective towers of $3 \times 5$ cells in the second layer of the calorimeter. These energy clusters are then matched to tracks that are reconstructed in the inner detector and extrapolated to the calorimeter. Clusters without matching tracks are directly classified as unconverted photon candidates. Clusters with matched tracks are considered as electron candidates. To recover photon conversions, clusters matched to tracks originating from reconstructed conversion vertices in the inner detector or to tracks consistent with coming from a conversion are considered as converted photon candidates. To increase the reconstruction efficiency of converted photons, also converted candidates where one of the two tracks is not reconstructed are retained (see Refs. [10] and [15] for more details on converted photon reconstruction). The final energy measurement is done with only the calorimeter for both converted and unconverted photons, using a cluster size which depends on the photon classification. In the barrel a size corresponding to $3 \times 5$ cells in the second layer is used for unconverted photons and $3 \times 7$ for converted photon candidates (to still collect most of the photon energy despite the opening between the conversion products in the $\phi$ direction in the magnetic field). In the end-cap a size of $5 \times 5$ is used for all candidates. A dedicated energy calibration [9] is then applied to account for upstream energy loss, lateral leakage and longitudinal leakage, separately for converted and unconverted candidates. Photon candidates with calibrated transverse energies above 10 GeV are retained for the successive analysis steps.

To ensure a proper identification, the cluster barycenter in the second layer of the electromagnetic calorimeter is required to lie in the $\eta$ region covered by the very finely segmented first layer, $|\eta|<1.37$ or $1.52 \leq|\eta|<2.37$. In addition, for this analysis, photon candidates are selected to be outside regions of the electromagnetic calorimeter where either the presampler or the first or second layers have non working readout optical links: the full $3 \times 7$ (in the barrel) or $5 \times 5$ (in the end-cap) clusters are required not to overlap with any of these regions. Photon candidates are also rejected if one of the core $3 \times 3$ second layer cells is not working properly or if one of the first layer cells facing the second layer hottest cell is not working. These requirements reject $5.5 \%$ of photon candidates in both data and Monte Carlo samples.

After this preselection, 268992 photon candidates remain in the data sample with transverse energies above 10 GeV . The transverse energy distribution of these candidates is shown in Fig. 2. This distribution is compared to the one predicted from the simulation, where both prompt photons (from the dedicated signal samples for the hard-scattering produced photon and from the QCD samples for the quark QED radiation contribution) and "fake" photons (from the QCD background samples) are included. For $E_{\mathrm{T}}$ above 20 GeV , the higher threshold QCD sample is used. For lower photon candidate energies, the lower
threshold QCD sample is used. It is clear that, at this level, the sample is dominated by "fake" photons. Since the simulation is not expected to accurately predict the fake rate and the background composition, the fake contribution has been normalized such that the sum of fake and prompt photons contributions matches the observed data yield for Figures 2-5. For example in Figure 2 this results in an overall factor of 0.45 applied to the absolute Monte Carlo normalization for the fake component.


Figure 2: Transverse energy distribution of photon candidates after reconstruction and preselection. The data are represented by dots, the histogram represents the expectations from Monte Carlo simulations. The simulated signal distribution (hollow histogram) is normalized to the data luminosity using the leading order PYTHIA cross section. The simulated background distribution is normalized such that the sum of fake and prompt photons (filled blue histogram) matches the observed data yield.

To discriminate signal from background, shape variables computed from the lateral and longitudinal energy profiles of the shower in the calorimeters are used. First, the leakage $\left(E_{\mathrm{T}, \mathrm{had}} / E_{\mathrm{T}}\right)$ in the first layer of the hadronic compartment beyond the electromagnetic cluster is required to be small (below $1-2 \%$ depending on the pseudorapidity of the photon candidate) compared to the cluster energy. Then, the transverse shape in the second layer of the electromagnetic calorimeter is inspected, using ratios of energy deposits in $3 \times 7$ over $7 \times 7$ cells $\left(R_{\eta}\right)$ and $3 \times 3$ over $3 \times 7$ cells $\left(R_{\phi}\right)$ in $\eta \times \phi$, and using the RMS width $\left(w_{\eta 2}\right)^{1}$ of the energy distribution in $\eta$. Examples of these variables are shown in Figure 3 for all the reconstructed photon candidates passing the preselection criteria previously described. The comparison between data and simulation is sensitive to the detailed composition of the background in the simulation, and to the knowledge of the upstream material before the calorimeter, and at smaller level to the modeling of cross-talk between calorimeter cells in the simulation. From these variables, a set of loose photon identification criteria is defined. They rely on simple rectangular cuts on the three variables $E_{\mathrm{T}, \mathrm{had}} / E_{\mathrm{T}}, R_{\eta}$ and $w_{\eta 2}$. The values of the cuts are the same for converted and unconverted candidates. They are independent of the photon candidate transverse energy but depend on its pseudorapidity: they

[^53]have been chosen in order to obtain an efficiency around $99 \%$ with respect to reconstruction for true prompt photons (both converted and unconverted ones) for transverse energies greater than 20 GeV [10].


Figure 3: Examples of discriminating shower shape variables based on the energy deposits in the second longitudinal compartment of the electromagnetic calorimeter for photon candidates with $|\eta|<0.6$. The data are represented by dots, the histograms represent the expectations from Monte Carlo simulations for true prompt photons (hollow white histogram) and all photon candidates from signal and background processes (filled blue histogram). For the normalization of the simulated distributions see caption of Fig. 2. Left: transverse shape variable $R_{\eta}$. Right: transverse shape variable $R_{\phi}$. Top: unconverted photon candidates. Bottom: converted photon candidates.

To reject further the background, the shower shape in the first layer of the calorimeter is examined. Several variables which discriminate single photon showers from overlapping nearby showers originating by photon pairs from neutral meson decays are computed from the energy deposited in the first layer:

- the total RMS width $w_{s, \text { tot }}$ of the energy distribution along $\eta$ over all the cells of the cluster,
- the asymmetry $E_{\text {ratio }}$ between the first and second maxima in the energy profile of the first layer along $\eta$ ( 1 when there is no second maximum),
- the energy difference $\Delta E$ between the second maximum and the minimum between the two maxima ( 0 when there is no second maximum),
- the fraction $F_{\text {side }}$ of the energy in seven cells centered around the first maximum which is not contained in the three core cells centered around the first maximum,
- the RMS width $w_{s 3}$ of the energy distribution computed with the three core cells.

The second and third variables provide rejection against cases where the two showers give separated energy maxima in the first layer. The last two variables provide rejection against cases where the two showers are merged in a wider maximum. Figure 4 illustrates the comparison between data and simulation, after the loose selection, for some of these first layer shower shape variables. After the loose selection, the relative fraction of background candidates originating from a single $\pi^{0}$ is increased, thus this comparison is less sensitive to the uncertainty on the composition of the remaining background. In the central region of the detector, for relatively low values of the pseudorapidity $(|\eta|<0.6)$, the various shower shape variables are rather well described by the simulation. At larger $|\eta|$, shower shapes in the data are systematically broader than in the simulation. The impact of this difference is assessed in the next section. Using the first layer variables, the second layer variable $R_{\phi}$ and tighter selection on the quantities (the second layer variables $R_{\eta}$ and $w_{\eta 2}$ and the leakage in the hadronic calorimeter) exploited in the loose selection, the final tight selection criteria for photon identification are defined. Similarly to the loose photon identification criteria, in the early stage of the ATLAS data taking it has been chosen to base the tight photon identification criteria on simple cuts on each of the discriminating variables, instead of using more refined but - at the present level of understanding of the detector performance - less robust multivariate techniques. The values of the cuts are independent of the photon candidate transverse energy but depend on its pseudorapidity. They have been optimized using samples of simulated signal and background events prior to data taking. Different criteria are applied to converted and unconverted photon candidates: they have been chosen in order to obtain an efficiency around $85 \%$ with respect to reconstruction for true prompt photons in both categories for transverse energies greater than 20 GeV [10]. 11890 photon candidates are selected in the data sample after the tight selection.

Isolation is also an important variable for prompt photon studies: the prompt photon signal is expected to be more isolated from hadronic activity than the fake background from $\pi^{0}$ (or other neutral hadrons), which comes from jet production where the $\pi^{0}$ is very unlikely to carry the full original jet energy. Also, because of the mixture of hard-scattering and bremsstrahlung contributions in the prompt photon signal, it is important to have a well modeled isolation variable that can be linked to the parton level isolation cut used in next to leading order QCD computations. For the study discussed here, the isolation variable is computed using calorimeter cells from both the electromagnetic and hadronic calorimeters, in a cone of radius 0.4 in the $\eta-\phi$ space around the photon candidate. The contributions from $5 \times 7$ electromagnetic calorimeter cells in the $\eta-\phi$ space around the photon barycenter are not included in the calculation. The small leakage from the photon outside this region, evaluated as a function of photon transverse energy on simulated samples of single photons (thus avoiding additional contributions from the underlying event), is then subtracted from the isolation variable. After this correction the isolation energy becomes independent of the photon transverse energy. To reduce uncertainties from underlying event modeling, the isolation is then further corrected using a method suggested in Ref. [16]. For each of two different pseudorapidity regions ( $|\eta|<1.5$ and $1.5<|\eta|<3.0$ ), low energy jets are used to compute an ambient energy density, which is then multiplied by the area of the isolation cone and subtracted from the isolation energy. After this correction, whose average size is around 0.5 GeV , the distribution of the isolation variable is centered at zero for photons from the hard-scattering, with fluctuations that are dominated by electronic noise from the calorimeter measurement. The different isolation distributions for signal and background candidates from the simulation, as well as the distribution of selected candidates in data, are shown in Figure 5 for reconstructed photon candidates passing the preselection and the loose identification criteria. In the following, photon candidates having isolation energies lower than 3 GeV are considered as "isolated". This criterion is expected to be $96 \%$ efficient for photons from the hard-scattering and slightly less efficient for photons from parton bremsstrahlung and fragmentation, which have more hadronic activity nearby that gives rise to the asymmetric positive tail of the prompt photon signal distribution in Figure 5. The same criterion is expected to reject $44 \%$ of


Figure 4: Examples of discriminating shower shape variables based on the energy deposit in the first longitudinal compartment of the electromagnetic calorimeter, for all photon candidates (converted and unconverted) passing the preselection and the loose identification criteria. The data are represented by dots, the histograms represent the expectations from Monte Carlo simulations for true prompt photons (hollow white histogram) and all photon candidates from signal and background processes (filled blue histogram). For the normalization of the simulated distributions see caption of Fig. 2. Left: $E_{\text {ratio }}$. Right: $F_{\text {side }}$. Top: photon candidates with pseudorapidity $|\eta|<0.6$. Bottom: photon candidates with pseudorapidity $1.8 \leq|\eta|<2.37$.
background candidates with transverse energy above 10 GeV . Photon candidates with isolation energies higher than 5 GeV are considered as "non-isolated".

## 5 Efficiency of the photon identification and trigger criteria

### 5.1 Photon identification efficiency

The efficiency of the photon reconstruction and identification criteria (excluding the trigger efficiency, which is determined directly on data), is determined from the hard-scattering photon PYTHIA Monte Carlo sample. The reconstruction and identification efficiency as a function of the true photon transverse energy, after the preselection criteria described in the previous section have been applied is shown in Figure 6 . The efficiency is slightly lower for photons from QED radiation which are less isolated.

To estimate the systematic uncertainties from the description of material before the calorimeter, dedicated single photon samples with different geometry layouts have been simulated. In these samples, additional dead material has been placed in the inner detector volumes, in the electromagnetic calorime-


Figure 5: Distribution of the isolation energy of reconstructed photon candidates passing the preselection and the loose identification criteria. The data are represented by dots, the histograms represent the expectations from Monte Carlo simulations for true prompt photons (hollow white histogram) and all photon candidates from signal and background processes (filled blue histogram). For the normalization of the simulated distributions see caption of Fig. 2.
ter cryostat and between the presampler and the first layer of the calorimeter. In the first case, inactive material has been added to the pixel system (from 1 to $4 \%$ of a radiation length at $\eta=0$ ), to the silicon microstrip detector (from 1 to $10 \%$ of a radiation length at $\eta=0$ ), and in the transition radiation detector (from 0 to $15 \%$ of a radiation length depending on $\eta$ ). The material in the cryostat and between the presampler and the first calorimeter layer have been increased by $10 \%$ and $5 \%$ of a radiation length, respectively. From these simulations, a $0.3 \%$ efficiency decrease per $1 \%$ radiation length material increase before the calorimeter is expected. From the a priori knowledge of the material before the calorimeter, uncertainties of a few $\%$ are then expected. The amount of cross-talk between calorimeter cells has also been varied in the simulation to estimate its impact on the photon efficiency which is found to be at the $2 \%$ level at $E_{\mathrm{T}}$ close to 10 GeV when the cross-talk is increased by $50 \%$.

Another approach consists in starting from the shower shape comparisons shown in the previous section for the background dominated candidates and to derive scale factors between data and simulation for each variable that can then be applied to the signal Monte Carlo samples. This approach is sensitive in addition to uncertainties in the background composition modeling, as well as to statistical uncertainties in the data. Typical effects of $5-10 \%$ on the efficiency are obtained this way. In the future, samples of clean electrons should provide a better check of the shower shape simulation and of the photon efficiency uncertainty.

The impact of the classification between converted and unconverted photon candidates is also studied varying the efficiency of correctly classifying converted photon candidates in the simulation and is found to be $1 \%$ on the overall efficiency for a $10 \%$ change in the efficiency to classify correctly converted photons.


Figure 6: Expected photon reconstruction and identification efficiency as a function of the true photon transverse energy, as obtained from a simulated sample of prompt photons produced in hard-scattering $\gamma$-jet events, for the loose (triangles) and tight (dots) selections.

### 5.2 Efficiency of the trigger selection

The efficiency of the L1 calorimeter trigger, relative to the photon reconstruction and offline selection, is estimated in two steps. First, using a prescaled sample of minimum bias triggers, the efficiency of a lower ( 2 GeV ) threshold L1 calorimeter trigger is determined. The measured efficiency, $\varepsilon=(99.88 \pm$ $0.11) \%$, is very close to $100 \%$ for reconstructed photon candidates with $E_{\mathrm{T}}$ above 10 GeV passing tight identification criteria. Then, using the sample of events passing the L 1 calorimeter trigger with a 2 GeV threshold, the efficiency of the higher ( 5 GeV ) threshold L1 calorimeter trigger, used for this analysis, is measured. The efficiencies with respect to the offline selection are computed for tight photon candidates as a function of the transverse energy. The results are shown in Figure 7.

The trigger efficiencies for transverse energies above 10 GeV are summarized also in Table 1, for loose and tight photon candidates. Monte Carlo samples are used to check the possible bias introduced by using photon candidates from data, which are a mixture of prompt and fake photons instead of only prompt photons. This bias, obtained from the absolute difference of the trigger efficiency for a pure signal simulated sample and a pure background simulated sample, is found to be smaller than $0.3 \%$ for tight photon candidates.

## 6 Background estimation and signal extraction

As the simulation cannot be trusted to predict accurately the fake rate, a data driven method is used to estimate the background and extract the prompt photon signal. This method relies on the use of the isolation variable and of the shower shape variables based on the energy measurement in the first layer of the electromagnetic calorimeter to define a two dimensional plane as illustrated in Fig. 8. We define the signal region as the region with isolated candidates (isolation energy lower than 3 GeV ) passing


Figure 7: Photon trigger efficiency with respect to the offline photon selection, as measured in data (circles) and simulated background events (triangles) on photon candidates passing the tight identification criteria.

Table 1: Trigger efficiency with respect to the offline photon selection for photons with transverse energies greater than 10 GeV . Only the statistical uncertainty is quoted. The systematic uncertainty is estimated to be smaller than $0.3 \%$ for tight photon candidates.

| $\|\eta\|$ interval | $\|\eta\|<0.6$ | $0.6 \leq\|\eta\|<1.37$ | $1.52 \leq\|\eta\|<1.8$ | $1.8 \leq\|\eta\|<2.37$ | All |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Efficiency (loose photons) [\%] | $99.71 \pm 0.03$ | $99.47 \pm 0.05$ | $98.33 \pm 0.12$ | $99.20 \pm 0.08$ | $99.32 \pm 0.03$ |
| Efficiency (tight photons) [\%] | $99.91 \pm 0.05$ | $99.87 \pm 0.05$ | $99.45 \pm 0.15$ | $99.70 \pm 0.13$ | $99.77 \pm 0.04$ |

the tight identification criteria, and three background enriched regions, two with non-isolated candidates (isolation energy greater than 5 GeV ) either passing or failing some of the first layer shower shape criteria of the tight selection, and one with isolated candidates not passing some of the first layer shower shape criteria. We define the number of candidates observed in data in the four regions as $N^{A}$ (signal region), $N^{B}$ (non-isolated candidates passing the shower shape requirements), $M^{A}$ and $M^{B}$ (candidates failing the shower shape criteria and which are respectively isolated or non-isolated). Assuming that the signal contribution in the three control regions is negligible, the observed numbers of candidates in these three regions ( $N^{B}, M^{A}$ and $M^{B}$ ) are due only to the background contribution. Assuming also that for the background the isolation (measured outside the cluster) is independent of the shape of the energy deposit in the cells of the first layer, the background rejection of the isolation requirement can be measured in the background control sample of candidates failing the first layer shower shape selection criteria from the ratio $M^{A} / M^{B}$, and then applied to the background yield in the non-isolated region passing the first layer shower shape cuts $\left(N^{B}\right)$ to obtain a data-driven estimate for the background yield in the signal region,


Figure 8: Illustration of the two-dimensional plane, defined by means of the isolation and a subset of the photon identification (ID) variables, used for estimating, from the observed yields $N^{B}, M^{A}$ and $M^{B}$ in the three control regions, the background yield in the signal region where the observed total yield is $N^{A}$.
$N_{\mathrm{bkg}}^{A}=N^{B} \times M^{A} / M^{B}$. The estimated signal yield $\left(N_{\text {sig }}^{A}\right)$ and purity $(P)$ in the signal region are therefore:

$$
\begin{align*}
N_{\mathrm{sig}}^{A} & =N^{A}-N^{B} \frac{M^{A}}{M^{B}}  \tag{1}\\
P & =1-\frac{N^{B}}{N^{A}} \frac{M^{A}}{M^{B}} \tag{2}
\end{align*}
$$

Provided the two assumptions above are satisfied, this method does not rely on any other inputs.
The choice of the shower shape variables to be used for the definition of the background control regions is driven by two main criteria. To minimize correlations between the isolation variable and the first layer variables, one would prefer to revert only the cuts on a small subset of shower shape variables that are less correlated with isolation in the background enriched samples. The natural choice would therefore be to revert the selection criteria on the two variables, $F_{\text {side }}$ and $w_{s 3}$, that use fewer cells from the first electromagnetic calorimeter layer, i.e. only the ones in the core of the cluster, thus expected to be the less correlated with the energy deposit outside the cluster. On the other hand, since the measurement presented here is significantly limited by the available statistics, and in particular the Poisson fluctuations of the data in the background control region, the more shower shape criteria are reverted the larger is the background in the control regions, which allows us to obtain a more precise extrapolation of the background in the signal region. A reasonable tradeoff has been found by reverting the requirements on four of the five shower shape variables (all but $w_{s, \text { tot }}$ ) for defining the background control regions. With this configuration, the correlation is computed in the background Monte Carlo sample and found to be typically lower than $15 \%$ in each of the twelve $\left(|\eta|, E_{\mathrm{T}}\right)$ bins under study. The values of the ratio $R=\frac{N_{\mathrm{bkg}}^{A} M_{\mathrm{bkg}}^{B}}{N_{\mathrm{bkg}}^{B} M_{\mathrm{bkg}}^{A}}$ integrated over the full pseudorapidity range are summarized in the first row of Table 2. The results of the measurement are then corrected in order to take into account residual non-zero correlations between the isolation and the shower shape variables as explained below. Moreover, the finite precision of this check will be taken into account as a systematic error on the background estimate.

The assumption that the signal contamination in the background control regions is small is checked using the prompt photon Monte Carlo sample. The control region most affected by signal is the one with isolated candidates failing the first layer shower shape cuts. The fraction of signal events which fall in this control region is found to be decreasing as a function of the photon transverse energy, from about $18 \%$ between 10 and 15 GeV to below $6 \%$ above 20 GeV (see Table 2). The three quantities $c_{i}$ represent the fractions of signal candidates in the three control regions relative to the signal yield in the signal region, and are obtained from simulated signal events. The fraction of signal events with respect to the total number of events in this control region is therefore expected to be around $5 \%$. This is then a small correction to the background extraction, which can anyway be taken into account explicitly in the formula for the estimated signal yield and purity as described in the following.

Table 2: Background pseudo-correlation factor $R=\frac{N_{\mathrm{bkg}}^{A} M_{\mathrm{bkg}}^{B}}{N_{\mathrm{bkg}}^{B} N_{\mathrm{bkg}}^{A}}$ and ratios $c_{1}=\frac{N_{\text {sig }}^{B}}{N_{\text {sig }}^{A}}, c_{2}=\frac{M_{\text {sig }}^{A}}{N_{\text {sig }}^{A}}$ and $c_{3}=\frac{M_{\text {sig }}^{B}}{N_{\text {sig }}^{A}}$ between the expected signal photons in the three control regions and the expected signal photons in the signal region, in different intervals of the reconstructed photon transverse energy.

| $E_{\mathrm{T}}$ interval $[\mathrm{GeV}]$ | $10 \leq E_{\mathrm{T}}<15$ | $15 \leq E_{\mathrm{T}}<20$ | $E_{\mathrm{T}} \geq 20$ |
| :--- | :---: | :---: | :---: |
| $R$ | $1.10 \pm 0.03$ | $0.91 \pm 0.05$ | $1.02 \pm 0.02$ |
| $c_{1}$ | $(1.8 \pm 0.2) \times 10^{-2}$ | $(3.1 \pm 0.5) \times 10^{-2}$ | $(5.3 \pm 0.3) \times 10^{-2}$ |
| $c_{2}$ | $(18.0 \pm 0.6) \times 10^{-2}$ | $(11.3 \pm 0.7) \times 10^{-2}$ | $(6.6 \pm 0.2) \times 10^{-2}$ |
| $c_{3}$ | $(5.3 \pm 1.1) \times 10^{-3}$ | $(2.5 \pm 1.3) \times 10^{-3}$ | $(6.9 \pm 1.0) \times 10^{-3}$ |

Since both the background correlation from the simulation and the signal leakage in the background control regions are found to be small but not negligible, they are accounted for in the background determination. The signal leakage in the three control regions is included by replacing, in Equation 1, the observed data yields with the yields corrected for the expected signal contribution, $N^{B} \rightarrow N^{B}-c_{1} N_{\text {sig }}^{A}$, $M^{A} \rightarrow M^{A}-c_{2} N_{\text {sig }}^{A}, M^{B} \rightarrow M^{B}-c_{3} N_{\text {sig }}^{A}$, and solving the resulting second order polynomial equation for $N_{\text {sig }}^{A}$. The correlations between the isolation and the shower shape variables are taken into account by correcting the estimated background yield in the signal region by the ratio between the true $\left(N_{\text {bkg }}^{A}\right)$ and the estimated $\left(N_{\mathrm{bkg}}^{B} \frac{M_{\mathrm{bkg}}^{A}}{M_{\mathrm{bkg}}^{B}}\right)$ background yield, obtained from simulated background events. The two corrections can be applied simultaneously in order to obtain the final measurement of the signal yield and purity in the signal region:

$$
\begin{align*}
N_{\mathrm{sig}}^{A} & =N^{A}-\left[\left(N^{B}-c_{1} N_{\mathrm{sig}}^{A}\right) \frac{M^{A}-c_{2} N_{\mathrm{sig}}^{A}}{M^{B}-c_{3} N_{\mathrm{sig}}^{A}}\right]\left(\frac{N_{\mathrm{bkg}}^{A}}{N_{\mathrm{bkg}}^{B}} \frac{M_{\mathrm{bkg}}^{B}}{M_{\mathrm{bkg}}^{A}}\right)  \tag{3}\\
P & =\frac{N_{\mathrm{sig}}^{A}}{N^{A}} \tag{4}
\end{align*}
$$

Figure 9(a) shows the distribution of the $F_{\text {side }}$ variable for the two regions "A", i.e. the isolated background control region and the signal region (full circles). Taking the shape of the background from the non-isolated background control regions (regions "B") and normalizing it to the number of events failing first layer shower cuts in the isolated sample (i.e. scaling it by $M^{A} / M^{B}$ ), the background in the isolated regions "A" is computed (open triangles). A clear excess at small $F_{\text {side }}$ can be observed which is consistent with the expected shape for the prompt photon signal (dashed histogram). Using the same technique, Figure 9(b) shows the total isolation energy distribution (full circles) and the background isolation distribution (open triangles), using the first layer variables to define the background enriched
control region and the signal region. Again a clear excess of isolated candidates in the sample fulfilling the first layer shower shape cuts can be seen.


Figure 9: (a) $F_{\text {side }}$ distribution for photon candidates with $E_{\mathrm{T}}>20 \mathrm{GeV}$ passing tight identification criteria (after releasing the criteria on $F_{\text {side }}, w_{s 3}, \Delta E$ and $E_{\text {ratio }}$ ), respectively belonging to the isolated (full circles) or non-isolated (open triangles) region. The latter have been scaled by the ratio $M^{A} / M^{B}$ defined in the text. (b) Isolation distribution for photon candidates with $E_{\mathrm{T}}>20 \mathrm{GeV}$ either passing the tight identification criteria (full circles), or passing the tight identification criteria after relaxing the requirements on four layer one shower shape variables (open triangles). The latter have been scaled by the ratio $N^{B} / M^{B}$ defined in the text. In both figures, the dashed line represent the prompt photon signal distribution, for candidates either passing the isolation (left) or identification (right) criteria. The signal has been normalized to the signal yield estimated in data in the signal region, divided by the expected efficiency of the identification or the isolation criteria, respectively.

The purity estimated with this method is shown in Fig. 10 in three different transverse energy bins, for four different pseudo-rapidity bins and averaged over the whole $|\eta|$ range. In this figure, only statistical uncertainties from the data and simulated samples are shown. The purity is clearly increasing with transverse energy, as expected from earlier simulation studies. The number of photon candidates in each $E_{\mathrm{T}}$ bin in the signal region in data, together with the estimated purity, are summarized in Table 3.

Table 3: Number of candidates in data, estimated signal purity and signal yield in the signal region (photon with isolation energy below 3 GeV and passing tight identification criteria), and corresponding systematic uncertainties, in three intervals of the photon transverse energy.

| $E_{\mathrm{T}}$ interval [GeV] | $10 \leq E_{\mathrm{T}}<15$ | $15 \leq E_{\mathrm{T}}<20$ | $E_{\mathrm{T}} \geq 20$ |
| :--- | :---: | :---: | :---: |
| Number of candidates | 5271 | 1213 | 864 |
| Estimated purity $P[\%]$ | $24 \pm 5$ | $58 \pm 5$ | $72 \pm 3$ |
| Systematic uncertainty on $P[\%]$ | 24 | 8 | 6 |
| Estimated signal yield $N_{\text {sig }}^{A}$ | $1289 \pm 297$ | $706 \pm 69$ | $618 \pm 42$ |
| Systematic uncertainty on $N_{\text {sig }}^{A}$ | 1362 | 86 | 59 |

In addition to the statistical uncertainty on the correction factors in Eq. 3 (the signal leakage fractions $c_{i}$ and the background pseudo-correlation factor $\frac{N_{\mathrm{bkg}}^{A}}{N_{\mathrm{bkg}}^{B}} \frac{M_{\mathrm{bkg}}^{B}}{M_{\mathrm{bkg}}^{A}}$, originating from the limited size of the simulated samples and included in the statistical uncertainty on the measured purity, the following effects are


Figure 10: Estimated prompt photon purity in data, as a function of photon transverse energy, for four different pseudo-rapidity bins and in the whole $|\eta|$ range. The points corresponding to the measurements in the full $|\eta|$ range (full circles) have been positioned, along the horizontal axis, at the average transverse energy of all selected photon candidates in the signal region in data, in the three intervals $10 \leq E_{\mathrm{T}}<15$ $\mathrm{GeV}, 15 \leq E_{\mathrm{T}}<20 \mathrm{GeV}$ and $E_{\mathrm{T}}>20 \mathrm{GeV}$ (identified by the dotted vertical lines). The points corresponding to the measurements in sub-intervals of the full $|\eta|$ range have been displaced arbitrarily along the horizontal axis for displaying purposes.
studied to investigate systematic uncertainties on the purity:

- The purity is evaluated after changing the isolation control region definition. The minimum isolation energy required for candidates in the non-isolated control regions, which is set to 5 GeV in the nominal measurement, is changed to 4 and 6 GeV . This would be sensitive to uncertainties in the contribution of prompt photons from QED quark radiation, which are less isolated than photons originating from the hard process. Alternative measurements are also performed where a maximum value of the isolation energy is set to 10 or 15 GeV for candidates in the non-isolated control regions, in order to reduce the correlation between the isolation variable and the shower shape distributions that is seen in simulated events in candidates belonging to the upper tail of the isolation distribution. The purity changes by at most $3.2 \%, 1.6 \%$ and $1.2 \%$ respectively for photons with transverse energies between 10 and 15 GeV , between 15 and 20 GeV and above 20 GeV .
- The number of shower shape variables that is used to define the background control region is reduced. This decreases the statistics of the background control sample but on the other hand should also reduce the correlation with the isolation variable. When using a subset formed by only the two variables ( $F_{\text {side }}$ and $w_{s 3}$ ) that are expected to be less correlated with the isolation variable, since they are computed with only the cells that are in the narrow core of the energy distribution
in the first layer of the calorimeter, the purity decreases by $21 \%$ in the low $E_{\mathrm{T}}$ bin and by less than $3 \%$ in the two $E_{\mathrm{T}}$ bins above 15 GeV .
- The systematics of the photon signal subtraction in the background control region is estimated using Monte Carlo samples with additional material before the electromagnetic calorimeter and additional cross-talk within the calorimeter cells. An upper limit of $5 \%$ on the fraction of signal photons being misidentified and therefore contributing the yields $M^{A}$ and $M^{B}$ observed in the two background control regions is derived. The purity, measured after varying the leakage coefficients $c_{2}$ and $c_{3}$ accordingly, changes by about $3.5 \%$ in all the $E_{\mathrm{T}}$ range. An additional source of uncertainty related to the signal subtraction originates from the different isolation distributions for the hard-scattering and bremsstrahlung signal photons, the latter being characterized by larger activity nearby and therefore by usually (slightly) larger values of the isolation energy. As a consequence, the fractions $c_{1}$ and $c_{3}$ of signal photons belonging to the non-isolated control regions and contributing to the observed yields $N^{B}$ and $M^{B}$ depend on the relative amount of prompt and bremsstrahlung photons in the selected sample. In the nominal measurement, we assume the fraction of hard-scattering photons in the signal region to be $60 \%$ of the total prompt photon signal as determined from simulation. We assign a systematic uncertainty on the purity due to this assumption by redoing the measurement after changing this fraction to $20 \%$ or $100 \%$. The measured value of the purity changes by $0.6,1.5$ and $2.4 \%$ respectively for photon with transverse energies between 10 and 15 GeV , between 15 and 20 GeV and above 20 GeV .
- The systematics from the uncertainty on the correlation in background events between the isolation energy and the shower shape variables used to define the four signal and background control regions is estimated by comparing the nominal purity measurement with the result obtained when neglecting completely this correlation (i.e. assuming $\frac{N_{\mathrm{bkg}}^{A}}{N_{\mathrm{bkg}}^{B}} \frac{M_{\mathrm{bkg}}^{B}}{M_{\mathrm{bkg}}^{A}}=1$ ). In addition, we perform again the purity measurement after varying the background pseudo-correlation factor by the difference (0.06) observed between our nominal simulated background sample and an alternative sample of $2 \rightarrow 2$ QCD hard-scattering events (excluding prompt photon production) generated with Herwig[17]. The purity result changes by at most $9.5 \%, 4.7 \%$ and $1.9 \%$ for photons with transverse energies between 10 and 15 GeV , between 15 and 20 GeV and above 20 GeV , respectively.
- The uncertainty on the electromagnetic energy scale, transported from test-beam measurements before in-situ determination, is $3 \% .^{2}$ We repeat the measurement after changing by $3 \%$, for each photon candidate, the cluster energy, the isolation and the cell energies used in the photon identification variables. The purity changes by at most $5 \%$, while the impact on the signal yield is higher (up to $25 \%$ between 10 and 15 GeV ).

The various systematic uncertainty sources and the corresponding uncertainties on the signal yield and purity in the three transverse energy intervals are summarized in Tables 4 and 5 . Combining the different effects above, we estimate the total systematic uncertainty on the purity to be between $24 \%$ and $6 \%$ as a function of transverse energy. The total systematic uncertainties for the purity measurements in each $E_{\mathrm{T}}$ bin are summarized in the last row of Table 3.

Some additional cross-checks have been performed to confirm the robustness of the method, but they have not been included in the systematic uncertainties:

[^54]Table 4: Systematic uncertainties on the estimated signal yield in three intervals of the photon transverse energy.

| $E_{\mathrm{T}}$ interval [GeV] | $10 \leq E_{\mathrm{T}}<15$ | $15 \leq E_{\mathrm{T}}<20$ | $E_{\mathrm{T}} \geq 20$ |
| :--- | :---: | :---: | :---: |
| Alternative non-isolated control region | 496 | 19 | 11 |
| Alternative non-identified control region | 1100 | 25 | 25 |
| Signal inefficiency of the identification criteria | 176 | 39 | 31 |
| Signal composition | 35 | 18 | 21 |
| Correlation between isolation and identification | 496 | 56 | 16 |
| Energy scale | 348 | 38 | 33 |
| Total | 1362 | 86 | 59 |

Table 5: Systematic uncertainties on the signal purity in three intervals of the photon transverse energy.

| $E_{\mathrm{T}}$ interval [GeV] | $10 \leq E_{\mathrm{T}}<15$ | $15 \leq E_{\mathrm{T}}<20$ | $E_{\mathrm{T}} \geq 20$ |
| :--- | :---: | :---: | :---: |
| Alternative non-isolated control region | 0.03 | 0.02 | 0.01 |
| Alternative non-identified control region | 0.21 | 0.02 | 0.03 |
| Signal inefficiency of the identification criteria | 0.03 | 0.03 | 0.04 |
| Signal composition | 0.01 | 0.02 | 0.02 |
| Correlation between isolation and identification | 0.10 | 0.05 | 0.02 |
| Energy scale | 0.05 | 0.05 | 0.01 |
| Total | 0.24 | 0.08 | 0.06 |

- The purity is measured separately for converted and unconverted samples. The total signal yield when summing both samples is consistent with the yield estimated from the combined sample within less than 0.4 times the statistical error on the signal yield (the total yield changes by $9 \%$ for transverse energies between 10 and 15 GeV , by $3.5 \%$ between 15 and 20 GeV , and by $1 \%$ above 20 GeV ). Above 15 GeV we have a clear evidence of both unconverted and converted photons: their yields are respectively $868 \pm 72$ and $425 \pm 49$ (including statistical error only, from data and from the limited size of the simulated samples). The purity for unconverted photons is about $10 \%$ higher than for converted ones. We note that the ratio between the converted and the unconverted signal yields for transverse energies above $15 \mathrm{GeV},(0.49 \pm 0.07)$, is in good agreement with Monte Carlo expectations $(0.45 \pm 0.01)$.
- The purity is measured separately in four pseudorapidity intervals, where the background level and the correlations between the isolation and the shower shape variables are expected to be different. The total signal yield when summing the yields in the four pseudorapidity ranges is consistent with that estimated from the combined sample within $10 \%$ or less of the statistical uncertainty on the signal yield (the total yield changes by $2.2 \%$ for transverse energies between 10 and 15 GeV , by $1.0 \%$ between 15 and 20 GeV , and by $0.2 \%$ above 20 GeV ).
- an alternative method which relies more finely on the shape of the isolation variable is used to estimate the purity. The isolation energy background distribution is subtracted from the observed distribution in data for photon candidates passing the tight identification criteria. The background template is obtained by scaling by the ratio $N^{B} / M^{B}$ the isolation energy distribution in a background enriched control data sample, formed by the photon candidates failing the tight criteria on the shower shape variables used to define the background control sample in the nominal measure-
ment. This method gives consistent results (always within at most $2 \%$, but typically within less than $1 \%$ in most of the $|\eta|$ and $E_{\mathrm{T}}$ bins) with those obtained from the simpler counting method used in this analysis when neglecting the signal in the background regions and neglecting correlations between the isolation and the identification variables in background.


## 7 Conclusion

A signal of prompt photon production has been extracted from a small set of $7 \mathrm{TeV} p p$ collision data collected at the LHC with the ATLAS detector. After tight identification cuts, a statistically significant prompt photon yield above 15 GeV is found, as well as a prompt photon purity which increases as a function of the photon transverse energy. For transverse energies above 20 GeV a signal yield of ( $618 \pm 72$ ) prompt photons with a purity of $(72 \pm 7) \%$ is measured, including statistical and systematic uncertainties. Together with the first estimates of the photon efficiency measurement, this gives confidence that a measurement of the prompt photon production cross section will soon be possible and that physics studies with photons in the final state are promising.

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# Search for the Higgs boson in the diphoton final state with $38 \mathbf{~ p b}^{-1}$ of data recorded by the ATLAS detector in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ 

The ATLAS collaboration


#### Abstract

This note reports on a search for the Standard Model Higgs boson in the diphoton decay channel with the ATLAS detector at a proton-proton center-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$, with an integrated luminosity of $38 \mathrm{pb}^{-1}$. In the Higgs mass range $110<m_{H}<140 \mathrm{GeV}$, the expected upper limit on the cross-section for this search is about 20 times larger than the Standard Model prediction. The observed exclusions range from 8 times the Standard Model prediction at 127 GeV , to 38 times at 116 GeV . A simulation-based study of signal, incorporating the best current knowledge of the detector performance, is presented and used in the limit setting.


## 1 Introduction

This note presents the first result of the ATLAS search for the Standard Model (SM) Higgs boson in the diphoton decay channel with the $38 \mathrm{pb}^{-1}$ of data collected in 2010 at a center-of-mass energy of 7 TeV . The general analysis strategy, the expected background estimation and the details of the data-driven background measurements follow closely the analysis described in [1]. The main goal of the previous work was to assess the background to this search with the first data taken in 2010. Despite the limited statistics, this measurement of the overall background is significantly more precise than all previous predictions based on simulation. Estimating the background directly in the data also allowed a consistent use of next-to-next-to-leading order (NNLO) cross sections for the signal compared to the background, since the simulation of backgrounds never reached this order in perturbative QCD . Based on the profile likelihood method introduced in [2,3] and used in [4], the exclusion limit on $H \rightarrow \gamma \gamma$ channel is set with current data. The impact of systematic uncertainties on the sensitivity is discussed.

## 2 Data sample

In comparison to the previous work [1], this analysis benefits from an improved estimation of the integrated luminosity [5], an additional $2 \mathrm{pb}^{-1}$ of recovered data, an improved photon identification which yields reduced systematic uncertainties, and finer-grained offline energy calibrations, evaluated with a sample of $Z \rightarrow e^{+} e^{-}$events, that improve the photon energy resolution and the corresponding uncertainties on the diphoton invariant mass resolution. The events are selected by a trigger which requires two photon candidates each with a transverse energy exceeding 15 GeV . In addition the events have to fulfill the criteria that the detector was fully operational. For the surviving events, at least two photon candidates in the central detector region with $p_{T}>25 \mathrm{GeV}$, and passing a loose photon identification criterion are required. Then kinematic cuts demanding transverse energy larger than 40 GeV and 25 GeV are applied on the leading and subleading photon candidates respectively. In addition tight photon identification and isolation criteria are applied [6]. The direction of the photon candidates is measured using the information from the first sampling of the electromagnetic calorimeter and on the measured position of the primary vertex. For events with more than one vertex reconstructed, the vertex associated with tracks having the highest sum of $p_{T}$ is used. The invariant mass is then deduced from the two photons with respect to this primary vertex. The final 2010 data sample has 99 events with a diphoton invariant mass between 100 and 150 GeV .

The number of diphoton, photon-jet and dijet events ( $N_{\gamma \gamma}, N_{\gamma j}+N_{j \gamma}$ and $N_{j j}$, where the first and second indices refer to the leading and subleading photon candidates, respectively) in the data sample are estimated by means of a double-sideband method, where the photon purity is evaluated by extrapolating to the signal region the background estimated from control regions located in the sideband plane of identification and isolation variables. The estimates of the sample composition are reported in Table 1, together with the predictions for the background components made in [7], corrected to take into account the effects of data quality, pile-up and the changes in the selection criteria. The contribution arising from Drell-Yan events is evaluated with a data-driven technique [1], and is not counted in the diphoton component. Figure 1 shows the diphoton invariant mass distribution, together with the predictions for the irreducible (diphoton) and reducible (photon-jet plus dijet) components of the backgrounds, and the composition estimated with the double-sideband method.

## 3 Signal modeling

At the LHC, there are several possible Higgs boson production processes, with cross sections calculated at different levels of precision. Monte Carlo (MC) samples for each subprocess, produced by the ATLAS

Table 1: The number of irreducible $\left(N_{\gamma \gamma}\right)$, reducible $\left(N_{\gamma j}+N_{j \gamma}, N_{j j}\right)$ and Drell-Yan $\left(N_{\mathrm{DY}}\right)$ background events to the $H \rightarrow \gamma \gamma$ search in the $100-150 \mathrm{GeV}$ mass range. For the measured number of events, the errors are statistical and systematic, respectively. For the expected number of events, the errors on the irreducible and reducible components arise from the theoretical uncertainty on the prediction; for the Drell-Yan component, the corresponding uncertainty arises from the MC statistics.

|  | $N_{\gamma \gamma}$ | $N_{\gamma j}+N_{j \gamma}$ | $N_{j j}$ | $N_{\mathrm{DY}}$ |
| :---: | :---: | :---: | :---: | :---: |
| Data | $75.0 \pm 13.3_{-3.6}^{+2.7}$ | $19.6 \pm 7.5 \pm 3.9$ | $1.5 \pm 0.7_{-0.5}^{+1.8}$ | $2.9 \pm 0.1 \pm 0.6$ |
| Expected | $86 \pm 23$ | $31 \pm 15$ | $1 \pm 1$ | $2.7 \pm 0.2$ |



Figure 1: Left: the diphoton invariant mass for the 99 events composing the data sample. The overlaid histograms represent the cumulative Drell-Yan (red solid), dijet (blue dotted), photon-jet (blue dashed) and diphoton (blue solid) components of the background, according to the predictions from theoretical models and simulation obtained in [7] and summarized in Table 1. The dark yellow band is the uncertainty for the reducible background components, and the yellow band is the total uncertainty on the reducible plus irreducible backgrounds. Right: the results of the double-sideband method for the 99 events composing the data sample. For the diphoton, photon-jet and dijet components, the extracted number of events on data (black dots) are compared with the corresponding predictions (yellow, mediumdark yellow and dark yellow bands, respectively). For the Drell-Yan component, the number of events is compared with the expected number of events predicted from simulation.
detector simulation package, and for values of the Higgs boson mass ranging from 110 to 140 GeV , are used to extract the efficiency of the signal reconstruction and the invariant mass resolution. Given the bunch structure and the instantaneous luminosities reached in 2010, the average number of proton-proton collisions per bunch-crossing was about 2.3. In order to mimic this effect, the MC event samples were produced with a configuration where the average number of interactions per bunch-crossing is equal to 2.2.

Table 2 summarizes the expected number of events from Higgs signals, as calculated from the Monte Carlo samples. The dominant uncertainties on the expected number of events, discussed in detail in Section 4 and summarized in Table 3, arise from the photon identification and isolation efficiencies and the theoretical uncertainties on the Higgs boson production cross-section [8].

The probability-density function (PDF) for the signal invariant mass is modeled by a Crystal Ball function (CB) (which takes into account the core resolution and a non-Gaussian tail extending towards
lower mass values) added to a small, wider Gaussian component (which takes into account outliers in the distribution). Figure 2 shows the invariant diphoton mass distribution for a sample of simulated events with a 120 GeV Higgs decaying into two photons and the PDF used to describe it. The resolution functions for Higgs at masses other than the simulated values are obtained through a linear interpolation of the PDF parameters.

Table 2: The expected Higgs signal yields for various mass points, for an integrated luminosity of 38 $\mathrm{pb}^{-1}$. The error combines the experimental systematic uncertainties and the theoretical uncertainty on the SM Higgs boson production cross-section [8].

| Higgs boson mass [GeV] | 110 | 115 | 120 | 130 | 140 |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Number of signal events | $0.43_{-0.09}^{+0.11}$ | $0.45_{-0.10}^{+0.11}$ | $0.45_{-0.10}^{+0.11}$ | $0.41_{-0.08}^{+0.10}$ | $0.31 \pm 0.08$ |



Figure 2: The distribution of the diphoton invariant mass for simulated events with a 120 GeV Higgs boson decaying into two photons. The data points are the output of the MC simulations. To reproduce the behaviour in data, the photon energy and resolution corrections described in Section 2 are applied on the invariant mass distribution. Furthermore, the fitted curve shows the PDF describing the invariant mass distribution; this represents also the resolution function used in the statistical analaysis described in Section 5. The FWHM of the distribution is 4.4 GeV .

The data points are the output of the MC simulations. To reproduce the behaviour in data the photon energy and resolution corrections described in Section 2 are applied on the invariant mass distribution. In addition, the fitted curve is shown.

## 4 Systematics

The background in the signal region is described with an exponential functional form using two nuisance parameters (a negative exponential coefficient and the overall normalization) which are fitted to the data.

The systematic uncertainties related to the signal can be divided into four main categories, and are summarized in Table 3. The first is the uncertainty on the luminosity which is common and correlated
among all Higgs decay channels. The second is the theoretical uncertainty on the overall normalization of the signal, dominated by the uncertainty on the computation of the production cross section as estimated in [8] (mostly due to scale dependence and uncertainties on the parton density functions). The third category corresponds to uncertainties on the efficiency, whose two main components are the uncertainty on the photon identification and on the isolation; these uncertainties are estimated from comparisons of data and fully simulated MC samples of photons and electrons. The fourth category of systematic uncertainties is on the invariant mass resolution. The contributions arising from uncertainties on the photon energy resolution are estimated using a fine-grained energy recalibration extracted from Z decays to electrons taking into account possible biases from the electron-to-photon extrapolation. An additional contribution arises from the impact of pile-up on the invariant mass resolution.

|  | Source | Uncertainty |
| :---: | :--- | :---: |
|  | Luminosity | $\pm 3.4 \%$ |
| Theory | Cross-section (scales) | ${ }_{-15}^{+20} \%$ |
| Efficiency | Photon identification | $\pm 11 \%$ |
|  | Photon isolation | $\pm 10 \%$ |
|  | Trigger | ${ }_{-3.7}^{+1.1} \%$ |
| Resolution | Calibration |  |
|  | $e \rightarrow \gamma$ extrapolation | $\pm 13 \%$ |
|  | Pile-up |  |

Table 3: Relative systematic uncertainties associated to the signal normalization and invariant mass resolution. For the resolution, the quoted uncertainty is relative to the width of the invariant mass.

Systematic uncertainties are treated by adding nuisance parameters and penalty PDFs that reflect the impact of these uncertainties in the likelihood function that is used in the definition of the test statistic. These penalty PDFs are in general simple Gaussian functions, with the exception of the trigger efficiency and theoretical cross-section, for which a double-sided Gaussian function is used.

## 5 Observed Sensitivity

The limits are set using a Power Constrained Limit (PCL) method. The procedure uses the profile likelihood ratio described in [2,3], with the p-value or $\mathrm{CL}_{s+b}$ extracted from the distribution of the profile likelihood ratio by toy MC. To protect against excluding the (signal) null hypothesis in cases of downward fluctuations of the background, the observed limit is not allowed to fluctuate below the $-1 \sigma$ expected limit. This is equivalent to restricting the statistical power of the analysis not to go below $16 \%$. This method is therefore referred to as the Power Constrained Limit $\mathrm{PCL}_{s+b}$. We therefore avoid showing the $-2 \sigma$ band in the resulting limit plot. Results using the $\mathrm{CL}_{s}$ (confidence level of excluding the signal hypothesis) method [9] are also provided as a reference.

Table 4 shows the upper bound on the exclusion at the $95 \%$ CL, in units of the SM Higgs boson cross-section, as a function of the Higgs boson mass for different methods. The systematic uncertainties introduced in Section 4 are taken into account in the limit setting by incorporating the corresponding penalty PDFs in the likelihood function used to model the data sample. On average, the incorporation of systematics degrades the exclusion limit by up to $10 \%$. With $38 \mathrm{pb}^{-1}$ of data, the obtained limits are mostly driven by statistical uncertainty, which explains the limited impact of systematic uncertainties. As expected, results from the $\mathrm{CL}_{s}$ methods are more conservative than those from the $\mathrm{CL}_{s+b}$ method.

Figure 3 shows the distribution of upper limits expected in the absence of any signal, indicated
by the median expected limit and $\pm 1 \sigma$ and $+2 \sigma$ contours, in addition to the observed limit. As the observed limit is constrained not to lie below the $-1 \sigma$ band for the expected limit, the $-2 \sigma$ band is not displayed in the plot. For Higgs masses around 127,132 and 140 GeV , the PCL constraint prevents a false exclusion due to a downwards background fluctuation. With an integrated luminosity of $38 \mathrm{pb}^{-1}$, this analysis shows that, in the median, cross-sections larger than about 20 times the prediction for the SM Higgs boson may be excluded. This limit is already comparable with recent results from Tevatron in the $H \rightarrow \gamma \gamma$ channel [10, 11, 12]. As a comparison, Figure 4 in Appendix A shows the observed exclusion computed with the $\mathrm{CL}_{s}$ method, for which the limits are around 5 units larger than the corresponding results using the $\mathrm{CL}_{s+b}$ method.

Table 4: Upper limits on the cross-section as a function of mass, in units of the SM prediction for the Higgs boson, at the $95 \% \mathrm{CL}$ for the $38 \mathrm{pb}^{-1}$ of data taken in 2010. $\mathrm{PCL}_{s+b}$ means the $\mathrm{CL}_{s+b}$ method with Power Constrained Limit technique for the computation of the observed limit. Results using $\mathrm{CL}_{s}$ are also provided as a reference.

| $\mathrm{m}_{H}[\mathrm{GeV}]$ | Expected limit |  | Observed limit |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $\mathrm{CL}_{s+b}$ | $\mathrm{CL}_{s}$ | $\mathrm{PCL}_{s+b}$ | $\mathrm{CL}_{s}$ |
| 110 | 22.1 | 27.9 | 16.1 | 24.0 |
| 115 | 20.1 | 25.5 | 37.9 | 39.7 |
| 120 | 19.9 | 24.4 | 23.6 | 27.2 |
| 130 | 19.1 | 24.0 | 9.3 | 18.3 |
| 140 | 23.0 | 29.9 | 8.0 | 20.7 |



Figure 3: The excluded Higgs production cross-section at the $95 \%$ CL, normalized by the SM prediction, as a function of the Higgs boson mass with $38 \mathrm{pb}^{-1}$ of data. The black solid line and the red dotted line correspond to the observed limit and expected limit, respectively. The green (yellow) band corresponds to the expected exclusion in the case of a $1 \sigma(2 \sigma)$ fluctuation of the background. The exclusion results are computed using $\mathrm{CL}_{s+b}$ with PCL.

## 6 Conclusion

In this note, the search for the $H \rightarrow \gamma \gamma$ search is reported with $38 \mathrm{pb}^{-1}$ data of proton-proton collisions at 7 TeV center-of-mass energy collected by the ATLAS experiment in 2010. Compared to [1], a modified photon identification and a set of finer-grained photon energy corrections are used in this analysis. The background to the $H \rightarrow \gamma \gamma$ signal is shown to be dominated by diphoton events. The study of the signal and systematics with current data are described. With the baseline $\mathrm{CL}_{s+b}$ method using the Power Constrained Limit technique for the observed exclusion, upper limits at the $95 \%$ Confidence Level are set on the cross-section for the $H \rightarrow \gamma \gamma$ process, in units of the expectation for the SM , as a function of the Higgs boson mass in the range $110-140 \mathrm{GeV}$. The exclusion limit ranges from 8 times the SM cross-section at $m_{H}=127 \mathrm{GeV}$ to 38 times the SM cross-section at $m_{H}=116 \mathrm{GeV}$. The expected limit based on CLs is comparable with recent results from the Tevatron in this channel [10, 11, 12].

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## Appendix A Results of exclusion with the $\mathbf{C L}_{s}$ method

Figure 4 shows the expected $1 \sigma$ and $2 \sigma$ exclusion intervals for the background-only test statistic in addition to the expected and observed exclusion limits. This method gives more conservative results than PCL in the region where the sensitivity to the signal is weak.


Figure 4: The excluded Higgs production cross-section at the $95 \%$ CL, normalized by the SM prediction, as a function of the Higgs boson mass with $38 \mathrm{pb}^{-1}$ of data. The black solid line and the red dotted line correspond to the observed limit and expected limit respectively. The green (yellow) band correspond to the expected exclusion in the case of $\mathrm{a} \pm 1 \sigma( \pm 2 \sigma)$ fluctuation of the background. The results are computed using the $\mathrm{CL}_{s}$ method.

## ATLAS NOTE

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# Jet energy scale and its systematic uncertainty in proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ with ATLAS 2010 data 

The ATLAS collaboration


#### Abstract

The jet energy scale (JES) and its systematic uncertainty are determined for jets measured with the ATLAS detector using $35 \mathrm{pb}^{-1}$ proton-proton collision data at $\sqrt{s}=7 \mathrm{TeV}$. Jets are reconstructed with the anti- $k_{t}$ algorithm with distance parameters $R=0.4$ and $R=0.6$, and are calibrated to the hadronic energy scale using Monte Carlo. The JES systematic uncertainty is evaluated for calorimeter jets with calibrated transverse momenta $p_{\mathrm{T}}^{\text {iet }}>20 \mathrm{GeV}$ and pseudorapidities $|\eta|<4.5$. It is estimated using a combination of insitu techniques and an analysis of systematic variations in Monte Carlo simulations, and it is found to be of similar size for both jet distance parameters studied. The smallest JES uncertainty of less than $2.5 \%$ is found in the central calorimeter region $(|\eta|<0.8)$ for jets with $60 \mathrm{GeV} \leq p_{\mathrm{T}}^{\text {jet }}<800 \mathrm{GeV}$. The JES uncertainty is the largest for low- $p_{\mathrm{T}}$ ( $20 \mathrm{GeV} \leq p_{\mathrm{T}}^{\text {jet }}<30 \mathrm{GeV}$ ) jets in the most forward region $3.2 \leq|\eta|<4.5$ where it amounts to $14 \%$. The additional energy due to multiple proton-proton interactions is corrected for and the remaining uncertainty is less than $1.5 \%$ per additional interaction for jets with $p_{\mathrm{T}}^{\text {jet }}>50 \mathrm{GeV}$ and decreases with $p_{\mathrm{T}}$. The JES is validated up to $p_{\mathrm{T}}^{\text {jet }}=1 \mathrm{TeV}$ using several in-situ methods.


## 1 Introduction

Over the course of the year 2010, the ATLAS detector [1] has been collecting data from proton-proton collisions at a center-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ delivered by the Large Hadron Collider (LHC). Understanding and measuring the performance of jets is crucial for many physics analyses at the LHC. The uncertainty of the jet energy calibration (jet energy scale, or JES) is the dominant experimental uncertainty for numerous physics results, for example the cross-section measurement of the inclusive jets, dijets and multijets [2-5], as well as vector boson accompanied by jets [6], and new physics searches with jets in the final state [7-10].

A first estimate of the JES uncertainty in the ATLAS detector was based on information available before the first LHC collisions and exploiting transverse momentum balance in di-jet events, and is described in Ref. [11]. An updated estimate of the JES uncertainty has been derived in Ref. [12] using in-situ measurements of the single hadron response [13,14]. These measurements allowed a significant reduction of the JES uncertainty in the central detector region. This note presents a further reduction of the JES systematic uncertainty in light of the increased knowledge of the detector performance gained during the analysis of the first year of ATLAS data [2,13-19] and results from the JES validation using in-situ techniques [20-22].

The estimate of the JES uncertainty described in this note follows closely the procedure described in Refs. [11, 12]. A reduction in the overall JES uncertainty is achieved thanks to more precise in-situ measurement of the calorimeter response to isolated hadrons and of the absolute electromagnetic energy scale of the calorimeters from the analysis of $Z$-boson decays in the electron channel $(Z \rightarrow e e)$.

The outline of the note is as follows: Sections 2-4 describe the ATLAS calorimeters, the Monte Carlo (MC) simulation framework, the event samples used for the estimate of the JES and the jet reconstruction procedure. Section 5 describes the jet calibration. It also details the jet selections applied to the Monte Carlo simulation samples used for the estimate of the jet energy scale and its uncertainty. Section 6 describes the sources of systematic uncertainties for the jet energy scale and their derivation using simulated and collision data. The effect of multiple proton-proton interactions (pile-up) that occur in addition to the event of interest on the jet energy measurement is discussed in Section 7. The combination of the individual uncertainty contributions is described in Section 8. A summary of the validation of the JES uncertainty using in-situ techniques is described in Section 9.

## 2 The ATLAS detector

The ATLAS detector consists of a tracking system (inner detector, or ID in the following) in a 2 T solenoidal magnetic field up to a pseudorapidity ${ }^{1}|\eta|<2.5$, sampling electromagnetic and hadronic calorimeters up to $|\eta|<4.9$, and muon chambers in a toroidal magnetic field. A detailed description of the ATLAS experiment can be found elsewhere [1].

Jets are reconstructed using the ATLAS calorimeter detectors, whose granularity and material varies as a function of $\eta$. The electromagnetic calorimeters employ liquid argon as the active material and lead for the accordion-shaped absorbers, and they cover up to $|\eta|<3.2$ (the barrel-endcap transition is at $1.37<|\eta|<1.52$ ). Liquid argon presamplers upstream of the electromagnetic calorimeter allow for corrections of the energy loss in front of the calorimeter due to the presence of the barrel solenoid and inner detector cryostat. The hadronic calorimeters make use of plastic scintillator and steel for the barrel and extended barrels (covering $0<|\eta|<0.8$ and $0.8<|\eta|<1.7$, respectively), and liquid argon and

[^55]copper for the endcaps $(1.5<|\eta|<3.2)$. The forward calorimeter is a liquid argon and tungsten/copper detector, and extends the calorimetry up to $|\eta|<4.9$.

## 3 Monte Carlo simulation of jets in the ATLAS detector

### 3.1 Event generators

Inclusive QCD jet events from proton-proton collisions at a center-of-mass of $\sqrt{s}=7 \mathrm{TeV}$ are generated using Pythia [23] 6.4.24 and Alpgen [24].

Pythia simulates non-diffractive proton-proton collisions using a $2 \rightarrow 2$ matrix element in leadingorder of the strong coupling to model the hard subprocess, and use parton showers to model additional radiation in the leading-logarithmic approximation. Mutliple parton interactions, as well as fragmentation and hadronisation are also simulated within PYthia. The parton distribution function (PDF) used for the Pythia samples is the modified leading order set MRST LO* [25].

ALPGEN is a leading order matrix-element generator for hard multi-parton processes in hadronic collisions. It is interfaced to the HERWIG generator [26] to produce parton showers in leading-logarithmic approximation. Parton showers are matched to the matrix element with the MLM matching scheme [27]. The hadronization is described by the cluster model also simulated within HERWIG. For the hadronization HERWIG is used and soft multiple parton interaction are modelled using Jimmy [28]. The PDF used for the Alpgen samples is CTEQ6L1 [29].

The parameters used for tuning the underlying event models in the Pythia and Alpgen event generators have been derived from minimum bias measurement in ATLAS data [30,31], and are denoted as ATLAS MC10 tune. No additional interactions within the same bunch crossing are simulated in any of the Monte Carlo samples used for the JES calibration and the determination of its uncertainty.

### 3.2 Simulation of the ATLAS detector

The Geant4 software toolkit [32] within the ATLAS simulation framework [33] propagates the generated particles through the ATLAS detector and simulates their interactions with the detector material. The energy deposited by particles in the active detector material is converted into detector signals with the same format as the ATLAS detector read-out. The detector signals are in turn reconstructed with the same reconstruction software as used for the data [33].

For the simulation of hadronic interactions in the detector, the GEANT4 set of processes called QGSP_BERT is chosen [34]. In this set of processes, the Quark Gluon String model [35] is used for the fragmentation of the nucleus, and the Bertini cascade model [36] for the description of the interactions of hadrons in the medium of the nucleus. The GEANT4 simulation and in particular the hadronic interaction model have been validated with test-beam measurements for the barrel [37-41] and the endcap [42-44] calorimeters. Further tests have been carried out in-situ using identified single particles from kaon and lambda decays produced in proton-proton collisions [45]. Excellent agreement between simulation and data has been found for pions and protons in the range of a few hundred MeV to 6 GeV , while the response of anti-protons is underestimated by about $10 \%$.

### 3.3 Nominal Monte Carlo simulation sample

The baseline (nominal) Monte Carlo sample used to derive the jet energy scale and to estimate the sources of its systematic uncertainty is composed by inclusive QCD jet events generated with the PYTHIA event generator and passed through the full ATLAS detector simulation. ATLAS jet data have been shown to be reasonably well described by PYthia MC simulations before and after jet calibration is applied [2, 13-19].

Studies of the material of the inner detector upstream the calorimeters have been performed using secondary hadronic interactions $[46,47]$. The ATLAS detector geometry used in the simulation of the nominal sample reflect the geometry of the detector as best known at the time of this study.

## 4 Jet reconstruction in the ATLAS detector

Jets are reconstructed using the anti- $k_{t}$ algorithm [48] with distance parameters $R=0.6$ and $R=0.4$ using the FastJet software [49, 50]. In the following, only anti- $k_{t}$ jets with distance parameter $R=0.6$ are discussed in detail. The results for jets with $R=0.4$ are similar unless stated otherwise. The fourmomentum recombination scheme is used.

The constituents of calorimeter jets are topological clusters (topoclusters) [51] that group together calorimeter cells. They are designed to follow the shower development taking advantage of the fine segmentation of the ATLAS calorimeters. The topocluster formation algorithm starts from a seed cell, whose signal-to-noise ratio (estimated as the energy deposited in the calorimeter cell over the RMS of the energy distribution measured in random events) is above a threshold of 4 . Cells neighboring the seed that have a signal-to-noise ratio of at least 2 are included iteratively, and finally all neighboring cells are added to the topocluster. The topoclustering algorithm also includes a splitting step: All cells in a cluster are searched for local maxima in terms of energy content, and the local maxima are then used as seeds for a new iteration of topological clustering, which will split the original cluster in more topoclusters. A topocluster is defined to have an energy equal to the energy sum of all the included cells, zero mass and a reconstructed direction as that of a unit vector originating from the center of the ATLAS coordinate system pointing to the energy-weighted topocluster barycenter.

Monte Carlo truth jets are reconstructed from the stable particles with a lifetime longer than 10 ps in the MC event record (excluding muons and neutrinos) using the same jet algorithm as for calorimeter jets. The four-momentum of a jet (before further calibration) is equal to the vectorial sum of the fourmomenta of its constituents.

## 5 Jet energy scale calibration

Jets are reconstructed at the electromagnetic scale, which is the basic signal scale for the ATLAS calorimeters. It accounts correctly for the energy deposited in the calorimeter by electromagnetic showers. This energy scale is established using test-beam measurements for electrons in the barrel [37,52-55] and endcap calorimeters [42,43]. The absolute calorimeter response to energy deposited via electromagnetic processes has also been validated in the hadronic calorimeters using muons, both from testbeams [37,56] and produced by cosmic-rays in-situ [57]. The energy scale of the electromagnetic calorimeters has been corrected using the invariant mass of $Z \rightarrow e e$ events from collision events ${ }^{2}$.

The goal of the jet energy scale calibration is to correct the energy and momentum of the jets measured in the calorimeter to those of the jet at the hadronic scale. The hadronic jet energy scale is on average restored using data-derived corrections and calibration constants derived from the comparison of the reconstructed jet kinematics to the one of the corresponding truth level jet in Monte Carlo studies. The jet energy scale calibration is then validated with in-situ techniques.

The jet calibration corrects for detector effects that affect the jet energy measurement:

1. partial measurement of the energy deposited by hadrons (calorimeter non-compensation),
2. energy losses in inactive regions of the detector (dead material),

[^56]3. energy deposits from particles not contained in the calorimeter (leakage),
4. energy deposits of particles inside the truth jet that are not included in the reconstructed jet,
5. signal losses in calorimeter clustering and jet reconstruction.

Presently, ATLAS uses a simple calibration scheme that applies jet-by-jet corrections as a function of the jet energy and pseudorapidity to jets reconstructed at the electromagnetic scale. This calibration scheme (called EM+JES) allows a direct evaluation of the systematic uncertainty and is therefore suitable for first physics analyses. The additional energy due to multiple proton-proton interactions within the same bunch crossings (pile-up) is corrected for before the hadronic energy scale is restored, so that the derivation of the jet energy scale calibration constants is factorised and does not depend on the number of additional interactions measured.

Other calibration schemes, described in Refs. [18,58], use additional cluster-by-cluster and/or jet-byjet information to reduce some of the sources of fluctuations in the jet energy response, thereby improving the jet resolution. These calibration techniques are presently undergoing commissioning in ATLAS.

The EM + JES calibration scheme consists of three subsequent steps as outlined below and detailed in the following sub-sections:

1. the average additional energy due to pile-up is subtracted from the energy measured in the calorimeters using correction constants extracted from an in-situ measurement,
2. the position of the jet is corrected such that the jet direction points to the primary vertex of the interaction instead of the geometrical centre of ATLAS detector,
3. the jet energy and position as reconstructed in the calorimeters are corrected using constants derived from the comparison of the kinematics of reconstructed jets and corresponding truth jets in Monte Carlo.

The calibration restores the jet energy scale within $2 \%$ for the full kinematic range, and a systematic uncertainty is assigned for the remaining non-closure as discussed in Section 6.2.

### 5.1 Pile-up correction

The energy of jets can include energy that does not come from the event of interest, but is instead produced by multiple proton-proton interactions within the same bunch crossing. A correction is derived from minimum bias data as a function of number of reconstructed primary vertices $N_{\mathrm{PV}}$ and jet pseudorapidity $\eta$, and takes into account the average additional energy deposited in a fixed grid of $0.1 \times 0.1$ in the $(\eta, \phi)$-plane (calorimeter towers) and the average number of such towers in a jet. This correction is applied at the electromagnetic scale as the first step of the calibration scheme. Further details on the pileup offset correction can be found in in Ref. [59]. The sensitivity of the jet energy resolution to pile-up has been studied and it has been found to be smaller than $1 \%$.

### 5.2 Jet origin correction

Calorimeter jets are reconstructed using the geometrical center of the ATLAS detector as reference to calculate the direction of jets and their constituents (see Section 4). The direction of each topocluster is corrected to point back to the primary vertex with the highest associated sum of track transverse momenta squared ( $\sum p_{T, \text { track }}^{2}$ ) in the event. The kinematics of each topocluster is recalculated using the vector from the primary vertex to the topocluster centroid as its direction. The raw jet four-momentum is thereafter redefined as the vector sum of the topoclusters four-momenta. This correction improves the angular resolution, resulting in a small improvement $(<1 \%)$ in the jet $p_{T}$ response. The jet energy is unaffected.

### 5.3 Final jet energy correction

The final step of the EM+JES jet calibration restores the reconstructed jet energy to the energy of the Monte Carlo truth jet. Since pile-up effects have already been corrected for, the Monte Carlo samples used to derive the calibration do not include multiple proton-proton interactions within the same bunch crossing.

The calibration is derived using all isolated calorimeter jets that have a matching isolated truth jet within $\Delta R=0.3\left(\Delta R=\sqrt{\Delta \eta^{2}+\Delta \phi^{2}}\right)$. Here, an isolated calorimeter (truth) jet is defined as a jet that has no other calorimeter (truth) jet with EM-scale (truth) $p_{T}>7 \mathrm{GeV}$ within $\Delta R=2.5 R$, where $R$ is the distance parameter of the jet algorithm. The EM-scale energy response $\mathcal{R}=E_{\text {calo }}^{\mathrm{EM}} / E_{\text {truth }}$ for each calorimeter-truth jet pair is measured in bins of the truth jet energy $E_{\text {truth }}$ and calorimeter jet detector pseudorapidity $\eta_{\text {det }}$, referring to the pseudorapidity of the original reconstructed jet before the origin correction. For each $\left(E_{\text {truth }}, \eta_{\text {det }}\right)$-bin, the measured EM-scale energy response $\langle\mathcal{R}\rangle$ is defined as the peak position of a Gaussian fit to the $E_{\text {calo }}^{\mathrm{EM}} / E_{\text {truth }}$ distribution, and the average calorimeter jet energy $\left\langle E_{\text {calo }}^{\mathrm{EM}}\right\rangle$ is determined. For a given $\eta_{\text {det }}$-bin $k$, a function $\mathcal{F}_{\text {calib, } k}\left(E_{\text {calo }}^{\mathrm{EM}}\right)$ of the jet response is obtained using a fit of the $\left(\left\langle E_{\text {calo }}^{\mathrm{EM}}\right\rangle_{j},\langle\mathcal{R}\rangle_{j}\right)$ points for each $E_{\text {truth }}$-bin $j$, where the fitting function is parameterised as:

$$
\begin{equation*}
\mathcal{F}_{\text {calib }, k}\left(E_{\text {calo }}^{\mathrm{EM}}\right)=\sum_{i=0}^{N_{\max }} a_{i}\left(\ln E_{\text {calo }}^{\mathrm{EM}}\right)^{i}, \tag{1}
\end{equation*}
$$

where $a_{i}$ are free parameters, and $N_{\max }$ is chosen between 1 and 6 depending on the goodness of the fit. The final jet energy scale correction that relates the measured calorimeter jet energy scale to the hadronic scale is then defined as $1 / \mathcal{F}_{\text {calib }, k}\left(E_{\text {calo }}^{\mathrm{EM}}\right)$ in the following:

$$
\begin{equation*}
E_{\text {calo }}^{\mathrm{EM}+\mathrm{JES}}=\frac{E_{\text {calo }}^{\mathrm{EM}}}{\mathcal{F}_{\text {calib }}\left(E_{\text {calo }}^{\mathrm{EM}}\right) \mid \eta_{\text {det }}}, \tag{2}
\end{equation*}
$$

where $\left.\mathcal{F}_{\text {calib }}\left(E_{\text {calo }}^{\mathrm{EM}}\right)\right|_{\eta_{\text {det }}}$ is $\mathcal{F}_{\text {calib,k}}\left(E_{\text {calo }}^{\mathrm{EM}}\right)$ for the relevant $\eta_{\text {det }}-$ bin $k$. The average jet energy scale correction $\left\langle 1 / \mathcal{F}_{\text {calib }, k}\left(E_{\text {calo }}^{\mathrm{EM}}\right)\right\rangle$ is shown as a function of calibrated jet transverse momentum $p_{\mathrm{T}}^{\text {jet }}$ for three jet $\eta$ intervals in Figure 1. The correction is only shown over the accessible kinematic range, i.e. values for jets above the kinematic limit are not shown. This is also the case for the following figures in this note. The calorimeter jet response $\mathcal{R}$ is shown for various energy- and $\eta_{\text {det }}$-bins in Figure 2. The value of the correction factor ranges from about 2.1 at low jet transverse momentum to less than 1.2 for high energy jets in the most forward region.

After the jet origin and energy corrections, the origin corrected jet $\eta$ is further corrected for a bias due to poorly instrumented regions of the calorimeter. In these regions topoclusters are reconstructed with a lower energy with respect to better instrumented regions (see Figure 2). This will cause the jet direction to be biased towards the better instrumented calorimeter regions.

The $\eta$-correction is derived as the average $\Delta \eta=\eta_{\text {truth }}-\eta_{\text {origin }}$ in $\left(E_{\text {truth }}, \eta_{\text {det }}\right)$-bins, and is parameterised as a function of the jet $E_{\text {calo }}^{\mathrm{EM}+\mathrm{JES}}$ and $\eta_{\text {det }}$. It is very small $(\Delta \eta<0.01)$ for most regions of the calorimeter but larger in the transition regions. The size of the bias is illustrated as a function of uncorrected detector pseudorapidity $\left|\eta_{\text {det }}\right|$ and EM + JES calibrated jet energy in Figure 3.

In the following, the EM+JES calibrated calorimeter jet transverse momentum will be denoted as $p_{\mathrm{T}}^{\text {jet }}$, and the corrected pseudorapidity simply as $\eta$.

## 6 Jet energy scale uncertainties

The JES systematic uncertainty is derived combining information from in-situ and single pion test-beam measurements, uncertainties on the material budget of the ATLAS detector, the description of the electronic noise, and the Monte Carlo modelling used in the event generation.


Figure 1: Average jet energy scale correction as a function of calibrated jet transverse momentum for three representative $\eta$-intervals. The correction is only shown over the accessible kinematic range, i.e. values for jets above the kinematic limit are not shown.

Dedicated Monte Carlo simulation test samples are generated with different conditions with respect to the nominal Monte Carlo sample described in Section 3.3. These variations are expected to provide an estimate of the systematic effects contributing to the JES uncertainty. The energy scale of jets for all the samples is calibrated using the calibration constants derived from the nominal Monte Carlo sample with the procedure described in Section 5.

The pseudorapidity bins used for the estimate of the JES uncertainty divide the ATLAS detector in the seven $\eta$ regions specified in Table 1.

Table 1: Detector regions and corrected pseudorapidity bins used for the estimate of the JES uncertainty.

| $\eta$ region | ATLAS detector regions |
| :---: | :---: |
| $0<\|\eta\| \leq 0.3$ | Central (Barrel) |
| $0.3<\|\eta\| \leq 0.8$ |  |
| $0.8<\|\eta\| \leq 1.2$ | Endcap |
| $1.2<\|\eta\| \leq 2.1$ | (Barrel-Endcap Transition and HEC) |
| $2.1<\|\eta\| \leq 2.8$ |  |
| $2.8<\|\eta\| \leq 3.2$ | Transition (HEC-FCal Transition) |
| $3.2<\|\eta\| \leq 3.6$ |  |
| $3.6<\|\eta\| \leq 4.5$ | Forward (FCal) |

The JES systematic uncertainty for all jets with pseudorapidity beyond $\eta=0.8$ is determined using the JES uncertainty for the central barrel region $(0.3<|\eta|<0.8)$ as a baseline, and adding a contribution from the relative calibration of the jets with respect to the central barrel region. This choice is motivated by the better knowledge of the detector geometry in the central region, and by the use of test-beam measurements only extending to the Tile calorimeter barrel for the estimate of the calorimeter response uncertainties.

This section focuses on the description of the sources of systematic uncertainties and their effect on


Figure 2: Simulated jet energy response at the electromagnetic scale as a function of EM +JES calibrated jet energy $E_{\text {calo }}^{\mathrm{EM}+\mathrm{JES}}$ and detector pseudorapidity $\eta_{\text {det }}$. Also shown are the $\eta$-intervals used to evaluate the JES uncertainty (see Table 1). The inverse of the response shown in each bin is equal to the average jet energy scale correction (and therefore equal to $\mathcal{F}_{\text {calib }}$ ).
the response of EM+JES calibrated jets. In Section 6.1, the selection of jets used to derive Monte-Carlo based components of the JES systematic uncertainty is outlined. The contributions to the JES systematics belonging to the categories below are then described:

1. the uncertainty due to the JES calibration method (Section 6.2);
2. the uncertainty due to the calorimeter response (Section 6.3);
3. the uncertainty due to the detector simulation (Section 6.4);
4. the uncertainty due to the physics model and parameters employed in the Monte Carlo event generator (Section 6.5);
5. the uncertainty due to the relative calibration for jets with $\eta>0.8$ (Section 6.6).

The JES systematic uncertainty is derived for isolated jets, while inclusive jets were considered in the previous uncertainty estimates $[11,12]$. This choice is motivated by the minor differences observed in the average kinematic jet response of the baseline QCD Monte Carlo samples and by the need to factorize the topology dependence of the close-by jet energy scale uncertainty for final states other than the QCD jets considered. The response of jets as a function of the distance to the closest reconstructed jet needs to be studied and corrected for separately if the measurement relies on the absolute jet energy scale. The additional uncertainty associated to close-by jets is discussed in Section 8.1.

### 6.1 Jet selection for the Monte Carlo based contributions to the JES uncertainty

The JES uncertainty components derived from Monte Carlo samples are obtained by studying the average calorimeter energy response of calibrated jets. This average response, defined as $\langle\mathcal{R}\rangle=\left\langle E_{\text {calo }}^{\mathrm{EM}+\mathrm{JES}} / E_{\text {truth }}\right\rangle$ or $\langle\mathcal{R}\rangle=\left\langle p_{\mathrm{T}}^{\text {jet }} / p_{\mathrm{T}}^{\text {truth }}\right\rangle$, is obtained by matching isolated calorimeter jets to MC truth jets as described in Section 5.3, but excluding the isolation cut for truth jets ${ }^{3}$. This is done separately for the nominal and

[^57]

Figure 3: Jet pseudorapidity bias as a function of the jet EM + JES calibrated calorimeter jet energy $E$ and uncorrected detector pseudorapidity $\left|\eta_{\text {det }}\right|$.
each of the alternative Monte Carlo samples. Only MC truth jets with $p_{\mathrm{T}}^{\text {truth }}>15 \mathrm{GeV}$, and calorimeter jets with a $p_{\mathrm{T}}^{\text {jet }}>7 \mathrm{GeV}$ after calibration, are considered. The calibrated response $\langle\mathcal{R}\rangle$ is studied in bins of truth jet transverse momentum $p_{\mathrm{T}}^{\text {truth }}$. The $p_{\mathrm{T}}^{\text {truth }}$ corresponding to the bin center is transformed on average to the calibrated $p_{\mathrm{T}}^{\text {jet }}$ value using a simple inversion procedure as described in Section 5.1 of Ref. [11]. The shifts between the Monte Carlo truth level $p_{\mathrm{T}}^{\text {truth }}$ bin centers and the reconstructed $p_{\mathrm{T}}^{\text {jet }}$ bin centers are negligible with respect to the chosen $p_{T}$ bin widths. Hence the average jet response can be obtained to good approximation as a function of $p_{\mathrm{T}}^{\mathrm{jet}}$.

### 6.2 Uncertainty due to the JES calibration

After the nominal inclusive jet Monte Carlo simulation sample is calibrated, the jet energy and $p_{T}$ response still shows slight deviations from unity at low $p_{T}$ (non-closure). This can be seen in Figure 4, showing the jet response for $p_{T}$ and energy as a function of $p_{\mathrm{T}}^{\text {jet }}$ for the nominal Monte Carlo sample in the barrel and endcap regions for anti- $k_{t}$ jets with $R=0.6$.

Any deviation from unity (non-closure) in $p_{\mathrm{T}}^{\mathrm{jet}}$ and energy response after the application of the JES to the nominal Monte Carlo sample implies that the kinematics of the calibrated calorimeter jet are not restored to that of the corresponding particle jets. This is mostly due to the following:

1. There is an underlying assumption that every constituent needs the same average compensation when deriving the calibration constants;
2. The same correction factor for energy and transverse momentum are used. In the case of a non-zero jet mass that does not reflect the truth jet mass, restoring only the jet energy and pseudorapidity will lead to a bias in the $p_{T}$ calibration.

The systematic uncertainty due to the non-closure of the nominal JES calibration is taken as the largest deviation of the response from unity between energy and $p_{\mathrm{T}}$. In the barrel region $0.3<|\eta|<0.8$ this contribution amounts to about $2 \%$ at low $p_{\mathrm{T}}^{\text {jet }}$ and smaller than $1 \%$ for $p_{\mathrm{T}}^{\text {jet }}>30 \mathrm{GeV}$. In the endcap and forward region, the closure is better than $1 \%$ for $p_{\mathrm{T}}^{\text {jet }}>20 \mathrm{GeV}$, while the energy response is within


Figure 4: Simulated jet $p_{T}$ response (full circles) after the EM + JES calibration and jet energy response (open squares) as a function of $p_{\mathrm{T}}^{\text {jet }}$ for the nominal sample for jets in the central (a), endcap (b) and forward (c) calorimeter regions.
$1 \%$ for jets with transverse momentum above 30 GeV . The deviation of the jet response from unity after calibration is taken as an additional source of systematic uncertainty.

### 6.3 Uncertainty on the calorimeter response

The response and corresponding uncertainties of single particles interacting in the ATLAS calorimeters can be used to derive the jet energy scale uncertainty in the central calorimeter region as detailed in Ref. [60]. The ATLAS simulation infrastructure allows for linking the true calorimeter energy deposits in each calorimeter cell to the particles generated in the collision. The uncertainty of the calorimeter response to jets can then be obtained from the response uncertainty of the individual particles constituting the jet. The in-situ measurement of the single particle response detailed in Ref. [60] significantly reduces the uncertainty due to the limited knowledge of the exact detector geometry, in particular those due to the presence of additional dead material, and the modelling of the interactions of particles in the detector.

The following single particle response measurements are used:

- the single hadron energy measured in a cone around an isolated track with respect to the track momentum $(E / p)$ in the momentum range from $0.5<p<20 \mathrm{GeV}$,
- the pion response measurements performed in the 2004 combined ATLAS test-beam, where a full slice of the ATLAS detector has been exposed to pion beams with momenta between 20 and 350 GeV [61].

Uncertainties for charged hadrons are estimated from these measurements as detailed in Ref. [60]. Additional uncertainties accounted for (see Sections 4.2 and 4.3 of Ref. [60]) include:

- effects related to the calorimeter acceptance,
- uncertainties related to particles with $p>400 \mathrm{GeV}$,
- baseline absolute electromagnetic scale for the hadronic and electromagnetic calorimeters for particles not measured in-situ,
- uncertainties connected to neutral hadrons.

At high transverse momentum, the dominating contribution to the calorimeter response uncertainties is due to particles with $p>400 \mathrm{GeV}$. The uncertainty for these particles has been conservatively estimated as $10 \%$ to take into account calorimeter non linearities and longitudinal leakage.

In the pseudorapidity range $0 \leq|\eta|<0.8$ the shift of the relative jet energy scale is up to $\approx 1 \%$, and the uncertainty on the shift is from 1 to $3 \%$. The total envelope (the shift added linearly to the uncertainty) of about $1.5-4 \%$ depending on the jet transverse momentum is taken as the relative JES calorimeter uncertainty.

### 6.4 Uncertainties due to the detector simulation

### 6.4.1 Calorimeter cell noise thresholds

As described in Section 4, topoclusters are constructed based on the signal-to-noise ratio of calorimeter cells, where the noise refers to (the RMS of) the measured cell energy distribution in events with no energy depositions from collision events. Discrepancies between the simulated noise and the real noise in data can lead to differences in the cluster shapes and to the presence of fake clusters, which affect the jet reconstruction. For data, the noise can change over time ${ }^{4}$, while the noise RMS used in the

[^58]simulation are fixed at the time of the production of the simulated data. This can lead to biases in the jet reconstruction and calibration if the simulated electronic noise injected in the Monte Carlo simulation does not reflect the noise in data.

The effect of the calorimeter cell noise (mis-)modelling on the jet response is estimated by reconstructing topoclusters, and thereafter jets, in Monte Carlo using the noise RMS measured in data. The actual energy and noise simulated in the MC are left unchanged, but the values of the thresholds used to include a given calorimeter cell in a topocluster are based on the cell noise RMS measured in data. The response of jets reconstructed with the modified noise thresholds are compared with the response of the jets reconstructed in exactly the same sample using the default MC noise thresholds. A series of cell noise thresholds values $(10 \%, 7 \%, 5 \%)$ were used to shift the noise thresholds for all cells (see Section 6.2 of Ref. [11] for details on this technique) to further study the effect on the jet response: increasing the cell thresholds in MC by $7 \%$ for each cell was found to give a similar shift in the jet response to using the noise RMS from data. Raising and lowering the cell thresholds by $7 \%$ shows that that the effect on the jet response from varying the cell noise thresholds is symmetric. This allows to use the calorimeter cell noise thresholds derived from data as a representative sample of the uncertainty on the jet energy scale. This covers both the case when more and less noise is present in data with respect to the simulation.

The maximal observed change in jet response is used to estimate the uncertainty on the jet energy measurement due to the calorimeter cell noise modelling. It is found to be below $3 \%$ for the whole pseudorapidity range, and negligible for jets with transverse momenta above 45 GeV . The uncertainties assigned to jets with transverse momenta below 45 GeV are:

- $1 \%$ and $2 \%$ for $20 \mathrm{GeV} \leq p_{\mathrm{T}}^{\mathrm{jet}}<30 \mathrm{GeV}$ for anti- $k_{t}$ with distance parameters $R=0.4$ and $R=0.6$ jets respectively,
- $1 \%$ for $30 \mathrm{GeV} \leq p_{\mathrm{T}}^{\text {jet }}<45 \mathrm{GeV}$.


### 6.4.2 Additional detector material

The jet energy scale is affected by possible deviations in the material description: the jet energy scale calibration has been derived to restore the energy lost under the assumption of the geometry simulated in the nominal Monte Carlo sample. Simulated detector geometries that include systematic variations to the material budget have been designed using test-beam measurements [53], in addition to 900 GeV and 7 TeV data $[46,47,62,63]$. Specific Monte Carlo samples have been produced using these distorted geometries.

In the case of uncertainties derived with in-situ techniques, such as those coming from the $E / p$ measurements detailed in Section 6.3, most of the effects on the jet response due to additional dead material are already taken into account because the measurement is performed directly on the ATLAS detector. However, The quality criteria on the track selection for the $E / p$ measurement effectively only allow particles that have not interacted in the inner detector to be included in the measurement. Therefore the effect of dead material in the inner detector needs to be taken into account for particles in the momentum range of the $E / p$ measurement. This is achieved using a specific Monte Carlo sample where the material budget is systematically varied adding $5 \%$ of material to the existing inner detector services. The uncertainty derived from the comparison of the distorted material response to the nominal response is then scaled by the fraction of particles within the $E / p$ momentum range. This uncertainty is shown in Figure 5.

Electrons, photons and hadrons with momenta $p>20 \mathrm{GeV}$ are not included in the $E / p$ measurements and therefore there is no in-situ estimate on the effect of any additional material in front of the calorimeters. This uncertainty is estimated using a dedicated Monte Carlo simulation sample where the overall detector material is systematically varied within the current uncertainties on the detector geometry knowledge. The overall changes in the detector geometry include:

- the increase in the inner detector material mentioned above;
- an extra 0.1 radiation length $\left(X_{0}\right)$ has been placed in the cryostat in front of the barrel of the electromagnetic calorimeter $(|\eta|<1.5)$;
- an extra $0.05 X_{0}$ has been placed between the presampler and the first layer of the electromagnetic calorimeter;
- an extra $0.1 X_{0}$ has been placed in the cryostat after the barrel of the electromagnetic calorimeter;
- extra material has also been placed in the in barrel-endcap transition region in the electromagnetic calorimeter ( $1.37<|\eta|<1.52$ ).

The uncertainty contribution due to the overall additional detector material is estimated by comparing the calibrated EM + JES jet response in the Monte Carlo sample with the distorted geometry with the nominal jet response (see Figure 5), and scaled by the average fraction of electrons, photons and high transverse momentum hadrons within a jet as a function of $p_{T}$.

### 6.5 Uncertainties due to the event modelling in the Monte Carlo generators

The contributions to the JES uncertainty from the modelling of the fragmentation and underlying event and other parameters of the Monte Carlo event generator are obtained using the following Monte Carlo samples:

- Alpgen + Herwig + Jimmy: the combination of the Alpgen generator interfaced to HERWIG and JIMMY is used to test the effects of a different modelling of the hard subprocess and soft processes. This configuration is tuned to ATLAS minimum bias data in a manner similar to the Pythia MC10 tune, and it has been described in Section 3.1. This model is different to the nominal Pythia sample in many respects, namely:
- the leading order matrix element calculation of multiple partons (legs) in the final state ( $2 \rightarrow 2$ to $2 \rightarrow 5$ for ALPGEN compared to $2 \rightarrow 2$ only for PYTHIA), and the matrix element matching to the parton shower with the MLM algorithm,
- the CTEQ6L1 parton distribution function used for Alpgen, compared to the MRST LO* set used for Pythia,
- the angular-ordered parton shower in HERWIG, compared with the $p_{T}$ ordered shower in Pythia,
- the cluster model for fragmentation implemented in HERWIG, compared to the PYTHIA string model,
- the underlying event implemented in JIMmy, compared to the PYthia model.
- Perugia2010 Pythia tune: this is an independent tune to the main hadron collider data with an increased final state radiation to better reproduce the jet shapes and hadronic event shapes using LEP and Tevatron data [64]. Also parameters sensitive to the production of particles with strangeness and related to jet fragmentation have been adjusted.

By comparing the baseline Pythia Monte Carlo sample to the Pythia Perugia2010 tune, the effects of soft physics modelling (e.g. underlying event) are tested. The Perugia2010 tune provides in particular a better description of the internal jet structure recently measured in ATLAS [4]. The Alpgen Monte Carlo uses different models for all phases of the event generation and therefore gives a reasonable estimate of


Figure 5: Simulated jet energy response (a) and $p_{\mathrm{T}}^{\mathrm{jet}}(\mathrm{b})$ response as a function of $p_{\mathrm{T}}^{\text {jet }}$ in the central region $(0.3<|\eta| \leq 0.8)$ in the case of additional dead material in the inner detector (full triangles) and in both the inner detector and the calorimeters (open squares). The response within the nominal Monte Carlo sample is shown for comparison (full circles).
the systematic variations. However, the possible compensation of effects that shift the jet response in opposite directions cannot be excluded.

Figure 6 shows the calibrated jet kinematic response for the two Monte Carlo generators and tunes used to estimate the effect of Monte Carlo theoretical model on the jet energy scale uncertainty, together with the kinematic response for the nominal sample shown for comparison. The ratio of the nominal response to the response for each of the two samples described is used to estimate a systematic uncertainty to the jet energy scale, and the procedure is detailed in Section 8.1.

### 6.6 Uncertainties due to the relative calibration in the endcap and forward regions

The JES uncertainty, determined in the central detector region using the single particle response and systematic variations of the Monte Carlo simulations, is transferred to the forward regions by exploiting the transverse momentum balance of a central and a forward jet in events with dijet topologies (where additional jets are vetoed as detailed in [65]). In such events, the responses of the forward jets are


Figure 6: Simulated energy response (a) and $p_{\mathrm{T}}^{\text {jet }}$ response (b) and as a function of $p_{\mathrm{T}}^{\text {jet }}$ in the central region $(0.3<|\eta| \leq 0.8)$ for Alpgen+Herwig+Jimmy (open squares) and Pythia with the Perugia2010 tune (full triangles). The response of the nominal Monte Carlo sample is shown for comparison (full circles).
measured relative to those of the central jets following a technique called "the matrix method" detailed in $[19,65]$. Measurements of this relative jet response are performed using the ATLAS 2010 data-set corresponding to an intergrated luminosity of $\approx 35 \mathrm{pb}^{-1}$, as well as using several MC generator event samples detailed in [65]. It is found that the MC predictions for the relative jet response diverge for low- $p_{\mathrm{T}}$ forward jets, while the data lie between the predictions.

These effects are accounted for in the uncertainty by including the intercalibration results for jets with $|\eta|>0.8$ in the total JES uncertainty as in the following:

- the total JES uncertainty in the central region $0.3<|\eta|<0.8$ is kept as a baseline,
- the uncertainty from the relative intercalibration is taken as the RMS deviation of the MC predictions from the data and is added in quadrature to the baseline uncertainty.

The intercalibration uncertainty is measured in bins of the average $p_{\mathrm{T}}$ of the two leading jets, labelled $p_{\mathrm{T}}^{\text {avg }}$. Due to momentum balance, this quantity is on average very similar to the average transverse
momenta of any of the two jets. The measurements are performed for transverse momenta in the range $20 \leq p_{\mathrm{T}}^{\text {avg }}<110 \mathrm{GeV}$. The uncertainty for jets with $p_{\mathrm{T}}>100 \mathrm{GeV}$ is taken as the uncertainty of the last available $p_{\mathrm{T}}$-bin. This is justified by the decrease of the intercalibration uncertainty with $p_{\mathrm{T}}$, but cannot completely exclude the presence of calorimeter non linearities for jet energies above those used for the intercalibration.

The uncertainties are evaluated separately for jets reconstructed with distance parameters $R=0.4$ and $R=0.6$, and are in general found to be slightly larger for $R=0.4$.

Figure 7 shows the relative jet response, and the associated intercalibration uncertainty calculated as detailed above, as a function of jet $|\eta|$ for two representative $p_{\mathrm{T}}^{\text {avg }}$-bins.


Figure 7: Jet $p_{\mathrm{T}}$ response measured relative to a central reference jet in data and various MC generator samples for jet $p_{\mathrm{T}}$ in the ranges $30-45 \mathrm{GeV}$ (left) and $80-110 \mathrm{GeV}$ (right). The resulting uncertainty component is shown as a shaded band around the data points.

## 7 Uncertainty due to multiple interactions

Particles produced by multiple soft proton-proton interactions in the same bunch crossing additional to the event of interest (in-time pile-up) can produce additional energy deposits that are reconstructed within the jet. As briefly described in Section 5, and fully detailed in Ref. [59], an average offset correction is applied to account for the average increase of the jet energy due to pile-up. This correction is parameterised as a function of the measured primary vertices $N_{\text {PV }}$.

The estimate of the remaining uncertainty on the jet energy scale after applying the pile-up correction is based on the studies described in Section 5 of Ref. [59]. The contributions to the uncertainty are estimated from studies that account for:

- the variation of the average offset-corrected calorimeter jet energy for calorimeter jets matched to track-jets as a function of the number of primary vertices,
- the effect of variations of the trigger selection on the measured tower energy distribution that is input to the offset correction,
- the mapping of the tower-based offset correction to a per-jet offset correction,
- the non-closure of the tower-based offset correction as evaluated by the dependence of the corrected calorimeter jet energy for calorimeter jets matched to track-jets as a function of the number of primary vertices.

The uncertainty on the jet energy scale is conservatively estimated by adding all uncertainties in quadrature, including the one from the non-closure of the correction. Since the track-jet method can be used only up to $|\eta|<1.9$ due to the limited coverage of the tracking detector, the di-jet balance method that is used for the $\eta$ intercalibration uncertainty and detailed in Section 6.6 have been used to estimate the uncertainty for $|\eta|>1.9$ by comparing the relative jet response in events with only one reconstructed vertex with the response measured in events with several reconstructed vertices. The dijet balance method yields uncertainties similar to those intrinsic to the method also in the case of $|\eta|<1.9$.

The offset correction and its uncertainty are derived as a function of the number of reconstructed vertices. This allows the correction and its uncertainty to be valid also for data periods where the number of reconstructed primary vertices is higher than the period where the correction is derived.


Figure 8: Relative pile-up uncertainty for anti- $k_{t}$ jets with $\mathrm{R}=0.6$ in the case of two measured primary vertices, $N_{\mathrm{PV}}=2$, for central $(0.3<|\eta| \leq 0.8$, full circles), endcap $(2.1<|\eta| \leq 2.8$, open squares) and forward ( $3.6<|\eta| \leq 4.5$, full triangles) jets as a function of jet $p_{\mathrm{T}}$.

Figure 8 shows the relative uncertainty due to pile-up in the case of two measured primary vertices. In this case, the uncertainty due to pile-up for central jets with $p_{T}=20 \mathrm{GeV}$ and pseudorapidity $|\eta| \leq 0.8$ is about $1 \%$, while it amounts to about $2 \%$ for jets with pseudorapidity $2.1<|\eta|<2.8$ and to less than $2.5 \%$ for all jets with $|\eta| \leq 4.5$. In the case of three primary vertices, the pile-up uncertainty is approximately twice that of $N_{\mathrm{PV}}=2$, and with four primary vertices the uncertainty for central, endcap and forward jets is less than $3 \%, 6 \%$ and $8 \%$, respectively. The relative uncertainty due to pile-up for events with up to 5 additional interactions becomes less than $1 \%$ for all jets with $p_{T}>200 \mathrm{GeV}$. The pile-up uncertainty needs to be added separately to the estimate of the total jet energy scale uncertainty detailed in Section 8.

The effect of additional proton-proton interactions from different bunch crossings that can be caused by trains of consecutive bunches (out-of-time pile-up) has been studied separately. The effect of out-oftime pile-up on jet reconstruction has been found to be negligible in the 2010 data-set.

## 8 Summary of the jet energy scale systematic uncertainty

### 8.1 Method to estimate the jet energy scale systematic uncertainty

The total jet energy scale uncertainty has been derived by considering all the individual contributions described in Section 6. In the central region $(|\eta|<0.8)$, the estimate proceeds as follows:

1. For each $p_{\mathrm{T}}^{\text {jet }}$ and $\eta$ bin, the uncertainty due to the calibration procedure is calculated as described in Section 6.2 for both jet energy and $p_{\mathrm{T}}$ response. For each bin, the maximum deviation from unity between the energy and $p_{\mathrm{T}}$ response is taken as the final non-closure uncertainty.
2. The calorimeter response uncertainty is estimated as a function of jet $\eta$ and $p_{T}$ from the propagation of single particle uncertainties to the jets, as detailed in Section 6.3.
3. Sources of uncertainties estimated using Monte Carlo samples with a systematic variation are accounted as follows:
(a) the response in the test sample $\mathcal{R}_{\text {var }}$ and the response in the nominal sample $\mathcal{R}_{\text {nom }}$ is considered as a starting point for the estimate of the JES uncertainty. The deviation of this ratio from unity is defined as:

$$
\begin{equation*}
\Delta_{\mathrm{JES}}\left(p_{T}^{\text {jet }}, \eta\right)=\left|1-\frac{\mathcal{R}_{\mathrm{var}}\left(p_{T}^{\text {jet }}, \eta\right)}{\mathcal{R}_{\mathrm{nom}}^{\text {jot }}\left(p_{T}^{\text {et }}, \eta\right)}\right| . \tag{3}
\end{equation*}
$$

This deviation is calculated from both the energy and $p_{T}$ response, leading to $\Delta_{\mathrm{JES}}^{\mathrm{E}}\left(p_{T}^{\text {jet }}, \eta\right)$ for the deviation in the energy response, and to $\Delta_{\mathrm{JTS}}^{\mathrm{pT}}\left(p_{T}^{\text {jet }}, \eta\right)$ for the deviation in the transverse momentum response.
(b) The largest $\Delta_{\mathrm{JES}}$ in each bin derived from the jet energy $(E)$ or transverse momentum ( $p_{T}$ ) response is considered as the contribution to the final JES systematic uncertainty due to the specific systematic effect:

$$
\begin{equation*}
\Delta_{\mathrm{JES}}\left(p_{T}^{\text {jet }},|\eta|\right)=\max \left(\Delta_{\mathrm{JES}}^{\mathrm{E}}\left(p_{T}^{\text {jet }}, \eta\right), \Delta_{\mathrm{JES}}^{\mathrm{pT}}\left(p_{T}^{\text {jet }}, \eta\right)\right) . \tag{4}
\end{equation*}
$$

4. The estimate of the uncertainty contributions due to additional material in the inner detector and overall additional dead material is estimated as described in point 3. above. These uncertainties are then scaled by the average fraction of particles forming the jet that are within $p<20 \mathrm{GeV}$ (for the inner detector distorted geometry) and by the average fraction of particles outside the $E / p$ in-situ measurements (for the overall distorted geometry).

For each $p_{\mathrm{T}}^{\text {jet }}, \eta$ bin, the contributions from the calorimeter, non-closure, Monte Carlo variations and dead material listed above are added in quadrature.

For pseudorapidities beyond $|\eta|>0.8$, the $\eta$ intercalibration contribution is estimated for each pseudorapidity bin in the endcap region as detailed in Section 6.6. The intercalibration contribution is added in quadrature to the total JES uncertainty determined in the $0.3 \leq|\eta|<0.8$ region to estimate the JES uncertainty for jets with $|\eta|>0.8$, with the exception of the non-closure term that is retained for the specific $\eta$ region. For low jet $p_{T}$, this choice leads to partially double count the contribution from the dead material uncertainty, but it is considered as a conservative estimate in a region where it is difficult to estimate the accuracy of the material description.

The contribution to the uncertainty due to additional proton-proton interactions described in Section 7 needs to be added separately, depending on the number of primary vertices in the event. In the following, only the uncertainty in the case of a single proton-proton interaction is shown in detail.

The jet energy scale has been derived using the simulated sample of QCD jets described in section 3.3, with a particular mixture of quark and gluon initiated jets and with a particular selection of isolated jets. The differences in fragmentation between quark and gluon initiated jets and the effect of close-by jets give rise to a particular topology and flavor dependence of the energy scale. Since the event topology and flavor composition (quark and gluon fractions) may be different in final states other than the QCD
jets considered, the dependence of the jet energy response on jet flavor and topology has to be accounted for in physics analyses.

The effect on the jet energy scale uncertainty due to close-by jets needs to be estimated separately, since the jet response depends on the angular distance to the closest jet. An additional analysis-dependent correction needs to be applied to jets with another jet close-by, and the additional uncertainty can be estimated from the Monte Carlo to data comparison of the $p_{T}$ ratio between calorimeter jets and matched track jets in inclusive dijet events as a function of the isolation radius. The analysis where this uncertainty is derived is described in Section 7 of Ref. [3]: it is found that simulated events reproduce the response of close-by-jets to within $1-3 \%$ as a function of the distance to the nearest jet, and an additional uncertainty is assigned.

As in the case of the topology dependence of the jet energy scale, specific flavor dependent corrections should be derived separately by different physics analysis. The systematic uncertainty will depend on the difference in the fraction of quark and gluon jets and on the flavor dependence of the jet energy response between data and simulation. This uncertainty has to be evaluated for each individual physics analysis.

### 8.2 Total jet energy scale systematic uncertainty

Figures 9,10 and 11 show the final fractional jet energy scale systematic uncertainty and its individual contributions as a function of jet $p_{\mathrm{T}}^{\mathrm{jet}}$ for three selected $\eta$ regions.

The fractional JES uncertainty in the central region amounts to 2 to $4 \%$ for $p_{\mathrm{T}}^{\mathrm{jet}}<60 \mathrm{GeV}$, and it is between 2 and $2.5 \%$ for $60 \mathrm{GeV} \leq p_{\mathrm{T}}^{\text {jet }}<800 \mathrm{GeV}$. For jets with $p_{\mathrm{T}}^{\text {jet }}>800 \mathrm{GeV}$, the uncertainty goes from 2.5 to $4 \%$, due to the larger uncertainties for particles with momentum beyond 400 GeV comprised in these jets. The uncertainty amounts to up to $7 \%$ and $3 \%$, respectively, for $p_{\mathrm{T}}^{\text {jet }}<60 \mathrm{GeV}$ and $p_{\mathrm{T}}^{\mathrm{jet}}>60 \mathrm{GeV}$ in the endcap region, where the central uncertainty is taken as a baseline and the uncertainty due to the relative calibration is added. In the forward region, a $13 \%$ uncertainty is present for $p_{\mathrm{T}}^{\text {jet }}<60 \mathrm{GeV}$ : the increase in the uncertainty is dominated by the modelling of the soft physics in the forward region that is accounted for in the intercalibration contribution.

The dominant contribution to the uncertainty for jets with the highest transverse momenta measurable in ATLAS is the calorimeter uncertainty, and more specifically the uncertainty due to particles in jets with $p>400 \mathrm{GeV}$. As stated in Section 6.3 and in [60], this uncertainty contribution is estimated conservatively.

Table 2 presents a summary of the maximum uncertainties in the different $\eta$ regions for anti- $k_{t}$ jets with distance parameter of $R=0.6$ and with $p_{\mathrm{T}}^{\text {jet }}$ of $20 \mathrm{GeV}, 200 \mathrm{GeV}$ and 1.5 TeV as an example.

The same study has been repeated for anti- $k_{t}$ jets with distance parameter $R=0.4$, and the estimate of the JES uncertainty is comparable to anti- $k_{t}$ jets with $R=0.6$. The JES uncertainty for anti- $k_{t}$ jets with $R=0.4$ is between $\approx 4 \%(8 \%, 14 \%)$ at low jet $p_{\mathrm{T}}^{\text {jet }}$ and $\approx 2.5-3 \%(2.5-3.5 \%, 5 \%)$ for jets with $p_{\mathrm{T}}>60 \mathrm{GeV}$ in the central (endcap, forward) region, and it is summarised in Table 3.

## 9 Validation using in-situ techniques

The jet energy calibration can be tested in-situ using a well calibrated object as reference and comparing data to the Pythia Monte Carlo simulation tuned to ATLAS data [30]. The following in-situ techniques have been used by ATLAS:

Direct transverse momentum balance between a jet and a photon [20]
Events with a photon and one jet at high transverse momentum are used to compare the jet transverse momentum to the one of the photon. To account for effects like soft radiation and energy


Figure 9: Fractional jet energy scale systematic uncertainty as a function of $p_{\mathrm{T}}^{\text {jet }}$ for jets in the pseudorapidity region $0.3 \leq|\eta|<0.8$ in the calorimeter barrel. The total uncertainty is shown as the solid light blue area. The individual sources are also shown, with uncertainties from the fitting procedure if applicable.


Figure 10: Fractional jet energy scale systematic uncertainty as a function of $p_{\mathrm{T}}^{\text {jet }}$ for jets in the pseudorapidity region $2.1 \leq|\eta|<2.8$. The JES uncertainty in the endcap region is extrapolated from the barrel uncertainty, with the uncertainty contribution from the $\eta$ intercalibration between central and endcap jets in data and Monte Carlo added in quadrature. The total uncertainty is shown as the solid light blue area. The individual sources are also shown, with uncertainties from the fitting procedure if applicable.


Figure 11: Fractional jet energy scale systematic uncertainty as a function of $p_{\mathrm{T}}^{\text {jet }}$ for jets in the pseudorapidity region $3.6<|\eta|<4.5$. The JES uncertainty for the forward region is extrapolated from the barrel uncertainty, with the uncertainty contribution from the $\eta$ intercalibration between central and forward jets in data and Monte Carlo added in quadrature. The total uncertainty is shown as the solid light blue area. The individual sources are also shown, with uncertainties from the fitting procedure if applicable.
migrating out of the jet area the data are compared to the Monte Carlo simulation. The comparison is done in the jet $\eta$ range $0 \leq|\eta|<1.2$ and for photon transverse momenta $25 \mathrm{GeV} \leq p_{\mathrm{T}}^{\text {jet }}<$ 250 GeV . The systematic uncertainties associated to the method itself are estimated to be about $1.5 \%$.

Photon balance using the missing transverse momentum projection [20]
The photon transverse momentum is balanced against the full hadronic calorimeter response using the projection of the missing transverse energy on the photon direction. This method does not involve explicitly a jet algorithm. The comparison is done in the same kinematic region as the direct photon balance method. The systematic uncertainty of the method is about $1 \%$.

Balance between a high- $p_{\mathrm{T}}$ jet recoiling against one or more lower- $p_{\mathrm{T}}$ jets [3]
If jets at low transverse momentum are well calibrated one can assess the calibration of jets at high transverse momentum by balancing against a recoil system of low transverse momentum jets. This method allows to probe the jet energy scale up to the TeV-regime. The $\eta$ range used for the comparison is $0 \leq|\eta|<2.8$. The systematic effects are evaluated to be about $4 \%$.

Comparison of jet calorimeter energy to the momentum carried by tracks associated to a jet [21] The mean transverse momentum sum of tracks that are within a cone with size R provide an independent test of the calorimeter energy scale over the total measured $p_{\mathrm{T}}^{\text {jet }}$ range within the tracking acceptance. The comparison is done in the jet $\eta$ range $0 \leq|\eta|<1.2$ and the systematic effects associated to the method are evaluated to be about $3 \%$.

The comparison of data to Monte Carlo simulation for all in-situ techniques are shown in Figure 12 together with the JES uncertainty for the $0 \leq|\eta|<1.2$ region as estimated from the single hadrons

Table 2: Summary of the maximum EM+JES jet energy scale systematic uncertainties for different $p_{\mathrm{T}}^{\mathrm{jet}}$ and $\eta$ regions from Monte Carlo-based study for anti- $k_{t}$ jets with $R=0.6$.

| $\eta$ region | Maximum fractional JES Uncertainty |  |  |
| :---: | :---: | :---: | :---: |
|  | $p_{T}^{\text {jet }}=\mathbf{2 0} \mathbf{~ G e V}$ | $p_{T}^{\text {jet }}=\mathbf{2 0 0} \mathbf{G e V}$ | $p_{T}^{\text {jet }}=\mathbf{1 . 5} \mathbf{~ T e V}$ |
| $0<\|\eta\|<0.3$ | $4.6 \%$ | $2.3 \%$ | $3.1 \%$ |
| $0.3<\|\eta\|<0.8$ | $4.5 \%$ | $2.2 \%$ | $3.3 \%$ |
| $0.8<\|\eta\|<1.2$ | $4.5 \%$ | $2.4 \%$ | $3.4 \%$ |
| $1.2<\|\eta\|<2.1$ | $5.5 \%$ | $2.5 \%$ | $3.5 \%$ |
| $2.1<\|\eta\|<2.8$ | $7.1 \%$ | $2.5 \%$ |  |
| $2.8<\|\eta\|<3.2$ | $8.5 \%$ | $3.0 \%$ |  |
| $3.2<\|\eta\|<3.6$ | $8.7 \%$ | $3.0 \%$ |  |
| $3.6<\|\eta\|<4.5$ | $12.6 \%$ | $2.9 \%$ |  |

Table 3: Summary of the maximum EM+JES jet energy scale systematic uncertainties for different $p_{\mathrm{T}}^{\mathrm{jet}}$ and $\eta$ regions from Monte Carlo based study for anti- $k_{t}$ jets with $R=0.4$.

| $\eta$ region | Maximum fractional JES Uncertainty |  |  |
| :---: | :---: | :---: | :---: |
|  | $p_{T}^{\text {jet }}=\mathbf{2 0} \mathbf{~ G e V}$ | $p_{T}^{\text {jet }}=\mathbf{2 0 0} \mathbf{G e V}$ | $p_{T}^{\text {jet }}=\mathbf{1 . 5} \mathbf{~ T e V}$ |
| $0<\|\eta\|<0.3$ | $4.1 \%$ | $2.3 \%$ | $3.1 \%$ |
| $0.3<\|\eta\|<0.8$ | $4.3 \%$ | $2.4 \%$ | $3.3 \%$ |
| $0.8<\|\eta\|<1.2$ | $4.3 \%$ | $2.5 \%$ | $3.5 \%$ |
| $1.2<\|\eta\|<2.1$ | $5.2 \%$ | $2.6 \%$ | $3.6 \%$ |
| $2.1<\|\eta\|<2.8$ | $8.2 \%$ | $2.9 \%$ |  |
| $2.8<\|\eta\|<3.2$ | $10.1 \%$ | $3.5 \%$ |  |
| $3.2<\|\eta\|<3.6$ | $10.3 \%$ | $3.7 \%$ |  |
| $3.6<\|\eta\|<4.5$ | $13.8 \%$ | $5.3 \%$ |  |

response and systematic variations of the Monte Carlo simulations. For the track-jet results the $\eta$ range used for the comparison in the figure is $0 \leq|\eta|<0.3$. The results of the in-situ techniques support the estimate of the JES uncertainty obtained using an independent method.

## 10 Conclusions

The jet energy scale uncertainty for jets produced in $p p$ collisions at a centre-of-mass energy of $\sqrt{s}=$ 7 TeV , and reconstructed with the anti- $k_{t}$ algorithm with distance parameters $R=0.4$ and $R=0.6$, has been estimated. The JES and its uncertainty are evaluated up to the kinematic limit (jet energies up to 3500 GeV ) and for calibrated jet pseudorapidities $|\eta|<4.5$.

Jets are calibrated in three subsequent steps starting from the electromagnetic scale measured in the calorimeter. First, additional energy due to multiple proton-proton interactions within the same bunch crossing is removed via an offset correction, then the jet origin is set to the primary collision vertex, and finally the jet energy scale and pseudorapidity are restored with calibration constants based on the true jet kinematics derived from the Monte Carlo simulation.

Compared to the previous jet energy scale uncertainty determination [11, 12], the uncertainty presented herein is significantly improved thanks to the reduced calorimeter response uncertainties. These


Figure 12: Jet energy scale uncertainty as a function of $p_{\mathrm{T}}^{\mathrm{jet}}$ in $0 \leq|\eta|<1.2$. This plot shows the data to Monte Carlo simulation ratios for several in-situ techniques that test the jet energy scale exploiting photon jet balance (direct balance or using the missing transverse momentum projection technique), the balance of a leading jet with a recoil system of two or more jets at lower transverse momentum (multijets) or using the momentum measurement of tracks in jets.
improvements are due to new measurements of the single hadron response, to a more detailed analysis of the uncertainties associated to neutral hadrons and to the recalibration of the electromagnetic scale of calorimeter with $Z \rightarrow e e$ events measured in-situ.

The total jet energy scale uncertainty decreases by up to a factor of two with respect to the update of the estimate in Ref. [12]. The jet energy scale calibration and the reduction in its uncertainty are validated by the comparison of calibrated jets in data and Monte Carlo simulation using in-situ techniques (tracks in jets, multi-jet balance, direct photon-jet balance, missing transverse energy projection fraction technique) up to jet transverse momenta of 1 TeV .

The jet energy scale uncertainty is found to be similar for jets reconstructed with both the jet distance parameters studied: $R=0.4$ and $R=0.6$. In the central region $(|\eta|<0.8)$ the uncertainty is lower than $4.6 \%$ for all jets with $p_{\mathrm{T}}>20 \mathrm{GeV}$, while for jet transverse momenta between 60 and 800 GeV the uncertainty is below $2.5 \%$.

In the endcap and forward region the relative intercalibration uncertainty dominates. The JES uncertainty amounts to a total of about $14 \%$ for the most forward pseudorapidities up to $\eta=4.5$.

The jet energy scale uncertainty is estimated for isolated jets, and similar results have been obtained using inclusive QCD jets. An additional correction due to the presence of close-by jets needs to be applied and an uncertainty of $1-3 \%$ added to the current estimate as a function of the distance to the nearest reconstructed jet. An additional flavour-dependent systematic uncertainty has to be evaluated for individual physics analyses.

The JES uncertainty due to proton-proton collisions occurring in addition to the event of interest (pile-up) after a dedicated correction is applied is estimated separately as a function of the number of primary vertices. In the case of two primary vertices per event, the uncertainty due to pile-up for jets with $p_{T}=20 \mathrm{GeV}$ and pseudorapidity $0.3 \leq|\eta|<0.8$ is about $1 \%$ while it amounts to about $2 \%$ for jets with pseudorapidity $2.1 \leq|\eta|<2.8$. For jets with transverse momentum above 200 GeV , the uncertainty due to pile-up is negligible $(<1 \%)$ for jets in the full pseudorapidity range $(|\eta|<4.5)$.

## Appendix A: additional jet energy scale uncertainty plots for comparison with ICHEP JES uncertainty

This section contains the JES uncertainty summary plots of section 8 for the central and endcap $\eta$ regions with the same axis range as Ref. [11] and Ref. [12].


Figure 13: Fractional jet energy scale systematic uncertainty as a function of $p_{\mathrm{T}}^{\mathrm{jet}}$ for jets in the pseudorapidity region $0.3 \leq|\eta|<0.8$ in the calorimeter barrel. The total uncertainty is shown as the solid light blue area. The individual sources are also shown, with statistical uncertainties if applicable.


Figure 14: Fractional jet energy scale systematic uncertainty as a function of $p_{\mathrm{T}}^{\text {jet }}$ for jets in the pseudorapidity region $2.1 \leq|\eta|<2.8$. The JES uncertainty in the endcap region is extrapolated from the barrel uncertainty, with the uncertainty contribution from the $\eta$ intercalibration between central and endcap jets in data and Monte Carlo added in quadrature. The total uncertainty is shown as the solid light blue area. The individual sources are also shown, with statistical uncertainties if applicable.

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## ATLAS NOTE

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# A Search for Randall-Sundrum Gravitons Decaying to Photon Pairs in $\sqrt{s}=7$ TeV pp Collisions 

The ATLAS Collaboration


#### Abstract

A search has been performed for evidence of a narrow resonance in the diphoton invariant mass spectrum. The analysis uses the ATLAS 2010 data set of proton-proton collisions at a center-of-mass energy of 7 TeV , produced by the CERN Large Hadron Collider, corresponding to an integrated luminosity of $36 \mathrm{pb}^{-1}$. No evidence of a narrow resonance above the Standard Model background is observed. The results exclude at $95 \%$ confidence level Randall-Sundrum graviton masses below $545 \mathrm{GeV}(920 \mathrm{GeV})$, for values of the dimensionless coupling $k / \bar{M}_{\mathrm{Pl}}$ of $0.02(0.1)$.


## 1 Introduction

The difference in the Standard Model (SM) between the Planck scale and the electroweak scale is known as the hierarchy problem. Recently, there has been great interest in models which resolve the hierarchy problem through the existence of extra spatial dimensions. One popular example is the Randall-Sundrum (RS) model [1], which postulates the existence of a fifth spatial dimension that has a "warped" geometry.

In the RS model, the 5 -dimensional spacetime is bounded by two ( $3+1$ )-dimensional branes. The particles of the SM are localized on one brane, while gravity is localized on the other. Given this spacetime configuration, TeV scales are naturally generated from the Planck scale due to a geometric "warp" factor:

$$
\begin{equation*}
\Lambda_{\pi}=\bar{M}_{\mathrm{Pl}} \exp \left(-k \pi r_{c}\right) \tag{1}
\end{equation*}
$$

where $\bar{M}_{\mathrm{Pl}}=M_{\mathrm{Pl}} / \sqrt{8 \pi}$ is the reduced Planck scale, and $k$ and $r_{c}$ are the curvature and compactification radius of the extra dimension, respectively. Given the exponential form of Eq. 1, the observed large hierarchy of scales is reproduced if $k r_{c} \approx 12$.

In the minimal RS model, gravitons are the only particles that can propagate in the bulk. As a result, a series of massive graviton excitations, known as a Kaluza-Klein (KK) tower, is predicted. These KK gravitons should have spin 2 , a mass splitting between successive KK levels on the TeV scale, and a universal dimensionless coupling $k / \bar{M}_{\mathrm{PI}}$ to the SM fields. The degrees of freedom of the RS model can be expressed in terms of $k / \bar{M}_{\mathrm{PI}}$ and the mass $M_{G}$ of the lightest KK graviton excitation. To address the hierarchy problem without the need for fine-tuning, $M_{G}$ should be in the TeV range. Coupling values in the range $0.01<k / \bar{M}_{\mathrm{Pl}}<0.1$ are favored, though values in the range $0.01<k / \bar{M}_{\mathrm{Pl}}<1.0$ have been considered in theoretical calculations [2].

A striking signature of the RS model at hadron colliders would be graviton production [2], followed by their decay to pairs of SM fermions or bosons. The graviton decay $G \rightarrow \gamma \gamma$ is a particularly interesting example, since observation of a resonance in the diphoton final state would rule out some possible alternative interpretations, such as a $Z^{\prime}$ boson. The production cross section of the diphoton final state is expected to be twice that of charged leptons, making this channel more sensitive to a potential graviton decay. For the ranges of graviton masses and couplings considered, the graviton would appear experimentally as a rather narrow resonance. The experimental backgrounds in the diphoton final state are relatively low, and the excellent energy resolution of the electromagnetic (EM) calorimeter would provide a good mass resolution. At a hadron collider, the leading production processes arise from $q \bar{q}$ annihilation and from gluon-gluon fusion, as depicted in Fig. 1, which shows leading order (LO) Feynman diagrams for graviton production and decay to the diphoton final state.


Figure 1: Leading order Feynman diagrams depicting RS graviton production at a hadron collider, followed by the decay $G \rightarrow \gamma \gamma$.

The most stringent existing limits on RS graviton production come from the D 0 experiment [3] at the Tevatron, which presented limits using $5.4 \mathrm{fb}^{-1}$ that combines results of the $G \rightarrow \gamma \gamma$ and $G \rightarrow e^{+} e^{-}$ channels. CDF has recently submitted to PRL the results [4] which they obtained from an analysis of the
$G \rightarrow \gamma \gamma$ final state using $5.4 \mathrm{fb}^{-1}$. The corresponding graviton mass limits from the Tevatron for values of $k / \bar{M}_{\mathrm{Pl}}=0.01$ and 0.1 are summarized in Table 1 .

| Value of <br> $k / \bar{M}_{\mathrm{Pl}}$ |  | 95\% CL Mass Limit (GeV) |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | D0 Expt | CDF Expt |  |  |
| 0.01 | 560 | 472 |  |  |
| 0.10 | 1050 | 976 |  |  |

Table 1: $95 \%$ CL lower limits on the RS graviton mass obtained by D0 [3] and CDF [4] for the values $k / \bar{M}_{\mathrm{Pl}}=0.01$ and 0.10 .

Given the larger center-of-mass-energy of the LHC, ATLAS should be able, even with relatively little integrated luminosity, to probe higher graviton masses than possible at the Tevatron. This note describes the analysis of the $G \rightarrow \gamma \gamma$ final state using $36 \mathrm{pb}^{-1}$ of data recorded by ATLAS in 2010.

## 2 Experimental Setup

The ATLAS detector [5] is a multipurpose particle physics apparatus with a forward-backward symmetric cylindrical geometry and nearly $4 \pi$ solid angle coverage ${ }^{1}$.

Closest to the beamline are tracking detectors which use layers of silicon-based and straw-tube detectors, located inside a thin superconducting solenoid that provides a 2 T magnetic field, to measure the trajectories of charged particles. The solenoid is surrounded by a hermetic calorimeter system. The liquid-argon (LAr) sampling calorimeter is divided into a central barrel calorimeter and two end-cap calorimeters, each housed in a separate cryostat. Fine-grained LAr EM calorimeters, with excellent energy resolution, provide coverage for $|\eta|<3.2$. In the region $|\eta|<2.5$, the EM calorimeters are segmented into three longitudinal layers and the second layer, in which most of the EM shower energy is deposited, is divided into cells of granularity of $\Delta \eta \times \Delta \phi=0.025 \times 0.025$. A presampler, covering $|\eta|<1.8$, is used to correct for energy lost upstream of the calorimeter.

An iron-scintillator tile calorimeter provides hadronic coverage in the range $|\eta|<1.7$. In the end-caps ( $|\eta|>1.5$ ), LAr hadronic calorimeters match the outer $|\eta|$ limits of the end-cap EM calorimeters. LAr forward calorimeters provide both EM and hadronic energy measurements, and extend the coverage to $|\eta|<4.9$. Outside the calorimeters is an extensive muon system including large air-core superconducting toroidal magnets.

## 3 Data and Monte Carlo Samples

The analysis uses the dataset collected in 2010 with the ATLAS detector at the LHC during stable beam periods of $p p$ collisions at a center-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$. The data were collected during the period from June through October 2010, and correspond to an integrated luminosity of $36 \mathrm{pb}^{-1}$.

Monte Carlo (MC) signal samples were produced using the implementation of the RS model in PYTHIA [6] version 6.424, which is fully specified by providing the values of $M_{G}$ and $k / \bar{M}_{\mathrm{Pl}}$. MC signal samples were produced for a range of $M_{G}$ and $k / \bar{M}_{\mathrm{Pl}}$ values. No background MC samples were used since we determine the expected number of background events from a data-driven method. The

[^59]MC samples used the MC09 parameter tune [7], and were processed through the ATLAS detector simulation [8] based on GEANT4 [9]. Some MC samples have been produced with a modified description of the detector material to study systematic effects. MC samples including multiple proton-proton collisions were produced, approximately reproducing the pile-up in data. Differences between data and MC are accounted for by re-weighting the simulated vertex multiplicity so that it matches the data.

## 4 Event Selection

Events selected for this analysis had to satisfy triggers that required the presence of photon candidates in the event. In the early running period, the only trigger requirement was that the first level ("Level-1") calorimeter trigger system identify at least one deposit of transverse energy above 14 GeV in the EM calorimeter with a shape consistent with an EM shower. Due to the moderate LHC collision rate in the first periods of data taking, the output rate for this trigger was low enough that no further trigger selection was needed. In later running, a diphoton trigger was used to cope with the increasing instantaneous luminosity delivered by the LHC. The diphoton trigger used a three level trigger which, at Level 1 , required at least two pairs of adjacent trigger towers with $E_{T}>10 \mathrm{GeV}$. The higher level trigger selection used a refined cluster reconstruction algorithm, in which the cluster is required to pass shower shape selections and to have $E_{T}>15 \mathrm{GeV}$. These trigger conditions were fully efficient for MC signal events which pass the offline reconstruction.

The data selection required at least one primary vertex candidate in the event, with at least three tracks associated to it. Events were required to also pass the ATLAS data quality requirements indicating that the relevant detectors were in working order during the given data taking period.

The reconstruction of photons is described in detail in Ref. [10]. To select photon candidates, EM calorimeter clusters were required to pass several quality criteria and to lie outside problematic calorimeter regions. Photon candidates were required to have $E_{\mathrm{T}}>25 \mathrm{GeV}$, to satisfy $|\eta|<2.37$ and to be outside the transition region $1.37<|\eta|<1.52$ between the barrel and end-cap calorimeters. The analysis uses a "loose" photon identification which includes cuts on the energy in the hadronic calorimeter as well as on variables that require the transverse width of the shower, measured in the second EM calorimeter layer, be consistent with the narrow width expected for an EM shower. The loose selection provides a high photon efficiency ( $\approx 94 \%$ ) with modest rejection against the background from jets. Finally photons were required to pass some quality selections to remove fakes initiated by noisy cells in the calorimeter and to avoid photons reconstructed close to regions of dead modules.

A total of 8090 events were selected with at least two photons that survived all analysis cuts. Of these, 1650 events have diphoton mass values above 120 GeV .

## 5 Background Description and Analysis Method

The main backgrounds for this analysis include the irreducible background from SM diphoton production, and reducible backgrounds from QCD $\gamma+$ jet and multijet events with at least one fake photon. The inclusive shape of the diphoton invariant mass distribution of the background is determined from a fit to a control region of masses between 120 and 500 GeV , which is a region in which the Tevatron results already exclude an RS graviton within the preferred range of values of $k / \bar{M}_{\mathrm{Pl}}(<0.1)$. When setting a limit for a 500 GeV graviton the background fit is restricted to the range between 120 and 430 GeV .

Figure 2 shows the diphoton candidate invariant mass spectrum in the control region. As expected, the background follows a smooth distribution. Superimposed on the figure is the result of a fit to the data of a sum of two exponential functions with freely varying parameters and relative strength. As seen from the figure, the background is described well by this parametrization; the p-value of the fit using a $\chi^{2}$ test is $94 \%$.


Figure 2: Diphoton candidate invariant mass distribution measured in the control region of 120 500 GeV . Superimposed is the result of a fit to the data of the background parametrization of the sum of two exponential functions.

To search for evidence of a resonance signal for a given graviton mass and coupling $k / \bar{M}_{\mathrm{P}}$, the observed invariant mass distribution within a window around the test mass was compared with histograms of the expected signal and background templates. The background prediction was determined by extrapolating the background fit function, with the parameters fixed to the values determined in the fit to the control region, into the search region of higher diphoton masses. The signal templates were determined from the signal MC samples, and include effects of both the natural graviton width and the experimental mass resolution.

One example of such templates for a 700 GeV graviton with $k / \bar{M}_{\mathrm{Pl}}=0.035$ is shown in Fig. 3. Each bin of the histograms is treated as a separate counting channel. Systematic uncertainties are included as nuisance parameters on the expected number of events with Gaussian distributions [11]. A given systematic uncertainty is taken as fully correlated across all bins of a histogram. The various systematic uncertainties are assumed to be uncorrelated with each other.

For each graviton mass, a different mass window was chosen for the search, in order to contain at least $90 \%$ of the signal in the window, including both the dependence of the resonance natural width on the value of $k / \bar{M}_{\mathrm{Pl}}$ and the $E_{T}$ dependence of the detector resolution. The chosen mass windows are given in Table 2, together with the expected number of signal and background events and the observed number of candidates.

## 6 Systematic Uncertainties

The various relative systematic uncertainties on the predicted RS graviton signal yield are summarized in Table 3. There is a $3.4 \%$ uncertainty on the integrated luminosity [12]. An uncertainty of $1 \%$ is attributed to the limited MC statistics and another $1 \%$ to the photon trigger efficiency. Uncertainties on the efficiency for reconstructing and identifying the $\gamma \gamma$ pair arise due to differences between MC and data in the distributions of the photon identification variables, the need to extrapolate these studies to the higher $E_{\mathrm{T}}$ values typical of the RS graviton signal photons, the impact of the photon quality

| G Mass [GeV] | $k / \bar{M}_{\mathrm{Pl}}$ | Mass Window [GeV] | $N_{\text {Exp }}^{S}$ | $N_{\text {Exp }}^{B}$ | $N_{\text {Obs }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 500 | 0.03 | $\pm 15$ | $12.8 \pm 2.1$ | $2.24 \pm 0.55$ | 3 |
| 550 | 0.03 | $\pm 30$ | $7.9 \pm 1.3$ | $5.5 \pm 2.3$ | 1 |
| 600 | 0.025 | $\pm 30$ | $3.4 \pm 0.6$ | $3.6 \pm 2.2$ | 3 |
| 650 | 0.04 | $\pm 30$ | $5.5 \pm 0.9$ | $2.4 \pm 1.7$ | 3 |
| 700 | 0.035 | $\pm 30$ | $2.8 \pm 0.5$ | $1.6 \pm 1.3$ | 2 |
| 750 | 0.05 | $\pm 35$ | $3.9 \pm 0.6$ | $1.2_{-1.1}^{+1.2}$ | 0 |
| 800 | 0.05 | $\pm 35$ | $2.6 \pm 0.4$ | $0.80_{-0.75}^{+0.98}$ | 1 |
| 850 | 0.06 | $\pm 40$ | $2.7 \pm 0.4$ | $0.60_{-0.60}^{+0.83}$ | 1 |
| 900 | 0.08 | $\pm 50$ | $3.4 \pm 0.6$ | $0.50_{-0.50}^{+0.84}$ | 2 |
| 925 | 0.085 | $\pm 55$ | $3.3 \pm 0.5$ | $0.45_{-0.44}^{+0.79}$ | 3 |
| 950 | 0.09 | $\pm 60$ | $3.1 \pm 0.5$ | $0.40_{-0.40}^{+0.75}$ | 3 |
| 975 | 0.11 | $\pm 70$ | $4.0 \pm 0.6$ | $0.38_{-0.38}^{+0.81}$ | 3 |
| 1000 | 0.13 | $\pm 90$ | $4.8 \pm 0.8$ | $0.42_{-0.41}^{+0.92}$ | 3 |
| 1025 | 0.13 | $\pm 90$ | $4.1 \pm 0.7$ | $0.34_{-0.33}^{+0.79}$ | 2 |
| 1050 | 0.13 | $\pm 90$ | $3.6 \pm 0.6$ | $0.27_{-0.27}^{+0.68}$ | 1 |
| 1100 | 0.15 | $\pm 110$ | $3.5 \pm 0.6$ | $0.23_{-0.23}^{+0.67}$ | 0 |
| 1150 | 0.15 | $\pm 115$ | $2.6 \pm 0.4$ | $0.16_{-0.16}^{+0.52}$ | 0 |
| 1200 | 0.2 | $\pm 165$ | $3.5 \pm 0.6$ | $0.18_{-0.17}^{+0.66}$ | 0 |
| 1250 | 0.2 | $\pm 165$ | $2.7 \pm 0.4$ | $0.11_{-0.11}^{+0.46}$ | 0 |

Table 2: Mass windows chosen to compute the $\mathrm{CL}_{\mathrm{s}}$ for each predicted graviton signal of a given mass and $k / \bar{M}_{\mathrm{Pl}}$ value. The expected number of signal $\left(N_{\text {Exp }}^{S}\right)$ and background ( $N_{\text {Exp }}^{B}$ ) events within the mass window are also shown, together with the number of observed data events ( $N_{\mathrm{Obs}}$ ). The errors shown are quadrature sums of the statistical and systematic uncertainties.


Figure 3: Expected signal (dashed) and background (solid), and observed (points) distributions in a mass window $\pm 30 \mathrm{GeV}$ around the resonance mass. The uncertainty on the signal and background is not shown in this illustration. The MC signal represents a 700 GeV graviton with $k / \bar{M}_{\mathrm{Pl}}=0.035$ and is normalized to the number of expected signal events for these parameter values.
selections, and uncertainties in the detailed material composition of the detector. Together these result in a systematic uncertainty of $3.8 \%$ on the efficiency for selecting diphoton events. The bunch-crossing uncertainty arises from the ability to determine the correct bunch crossing when pulse saturation occurs in the trigger digitization. This gives a systematic uncertainty of $2.0 \%$. The influence of pile-up gives a systematic uncertainty of $3.6 \%$.

While the previous uncertainties contribute to an uncertainty on the graviton signal yield, there are other sources of uncertainties that affect the shape of the diphoton candidate invariant mass distribution. The uncertainty on the photon energy resolution and energy scale impact the expected signal shape. Similarly, uncertainties in the determination of the background shape in the control region, and the extrapolation into the signal region, affect the background shape.

The photon energy scale and resolution systematics were determined by changing the signal MC templates. For the photon energy scale, shifts of $\pm 3 \%$ were applied to the photon $E_{\mathrm{T}}$ scale in signal MC events. The resolution was smeared by modifying the constant term in the resolution by $100 \%$ ( $400 \%$ ) for photons in the barrel (end-cap) calorimeter. In addition, a $20 \%$ smearing of the sampling term was applied. These uncertainties reflect the current understanding of the EM calorimeter calibration and reconstruction.

In order to study the systematic uncertainty attributed to the background tails which might not be correctly described by the extrapolation function, the background parametrization was fit to data in different ranges of the diphoton invariant mass. For a given test mass the fit was performed up to 100 GeV away from the test mass in steps of 100 GeV . The largest difference in the expected number of events from these various fits and the nominal fit up to 500 GeV was taken as the systematic uncertainty of the fit extrapolation and added in quadrature to the statistical uncertainty. The result of the background extrapolation uncertainty as a function of diphoton candidate invariant mass is shown as the brown band on Fig. 4.

The statistical uncertainty on the background shape extrapolation was determined by considering the statistical uncertainty on the background fit parametrization. To determine this effect, pseudoexperiments were performed by varying each bin in the control region according to a Poisson distribution around the measured value, refitting the so-obtained pseudo-data sample, and determining the fluctuation of the expected number of background events within the fit window. The $\pm 1(2)$ standard deviation bands were then determined by taking the integral of the spread of background around the nominal value such that $68 \%$ ( $95 \%$ ) of events were contained within the range. The statistical and systematic uncertainties determined are represented by green and yellow bands on Fig. 4.

The MRST2007lomod parton distribution function (PDF) set [13] has been used to determine the cross section of the graviton signals with PYTHIA. In order to estimate the systematic uncertainties due to the choice of PDF, the MSTW2008lo90cl PDF [14] set was used to change the value of the 20 eigenvalues by $\pm 1 \sigma$. The uncertainty coming from the PDF was estimated using the difference given by the modified PDF sets and the central value. The systematic uncertainty increases with the mass of the graviton. The uncertainty varies from $5.2-9.2 \%$ for masses between $500-1250 \mathrm{GeV}$. The systematic uncertainty due to the factorization and renormalization scales was estimated by changing the scale from the nominal value of 1 to 0.5 and 2 . This modification has at most a $6 \%$ effect on the graviton signal cross section.

| Source | Uncertainty (\%) |
| :--- | :---: |
| Luminosity | 3.4 |
| MC statistics | 1.0 |
| Photon trigger | 1.0 |
| Photon efficiency and ID | 3.8 |
| Photon quality | 0.5 |
| Bunch crossing ID | 2.0 |
| Pile-up | 3.6 |
| Photon energy resolution | Shape |
| Photon energy scale | Shape |
| PDF | $5.2-9.2$ |
| Fact. and renorm. scales | 6.0 |

Table 3: Summary of systematic uncertainties attributed to signal. The ones labeled 'Shape' involve modification of the signal templates.

## 7 Results

The invariant mass spectrum for diphoton candidates passing the selection cuts including loose photon identification is shown in Fig. 4 for the full mass range above 120 GeV . Superimposed is the result of the fit to the background in the control region below 500 GeV , which has been extrapolated to higher masses using the result of the fit. Also shown are graviton signals of masses 550, 700 and 1000 GeV and couplings $k / \bar{M}_{\mathrm{Pl}}=0.03,0.05$ and 0.11 , respectively. The three highest mass objects around 1000 GeV do not pass a more stringent photon selection that is designed to reduce the background due to jets, and are likely to be fake photon candidates. In fact, the highest mass diphoton candidate that passes the more stringent selection has a diphoton invariant mass of 679 GeV . An event display of this candidate is shown in Fig. 5.

The data are found to be well described by the smooth background parametrization over the entire


Figure 4: Reconstructed $m_{\gamma \gamma}$ distribution for data (points) and expected background (red line). Also shown are graviton signals of masses 550,700 and 1000 GeV and couplings $k / \bar{M}_{\mathrm{Pl}}=0.03,0.05$ and 0.11 , respectively. The signal is normalized to the number of expected events in an integrated luminosity of $36 \mathrm{pb}^{-1}$.


Figure 5: An event display of the highest invariant mass diphoton event in which both candidate photons satisfy the more stringent photon identification cuts. The highest transverse momentum photon has $\mathrm{p}_{\mathrm{T}}=194 \mathrm{GeV}$ and $(\eta, \phi)=(-1.32,-0.44)$. The trailing photon has $\mathrm{p}_{\mathrm{T}}=173 \mathrm{GeV}$ and $(\eta, \phi)=(1.10,2.82)$. The diphoton invariant mass is equal to 679 GeV .
mass range, and there is no evidence of a narrow resonance. For example, the p -value returned from evaluation of the spectrum using the BumpHunter tool [15] is $9 \%$, indicating agreement between the data and the background-only hypothesis.

Therefore, limits on graviton production were set using a log-likelihood ratio (LLR) defined as LLR $=-2 \ln (L($ data| $\mathrm{s}+\mathrm{b}) / L($ data $\mid \mathrm{b}))$ as the test statistic, where $L($ data| $\mathrm{s}+\mathrm{b})$ is the likelihood of the data using the signal plus background hypothesis and $L$ (data|b) is the likelihood of the data using the background only hypothesis.

The modified frequentist method [16] is used to determine the limit by performing pseudo-experiments to calculate $\mathrm{CL}_{\mathrm{s}+\mathrm{b}}=P\left(\mathrm{LLR} \geq \mathrm{LLR}_{\mathrm{obs}} \mid \mathrm{s}+\mathrm{b}\right)$ and $\mathrm{CL}_{\mathrm{b}}=P\left(\mathrm{LLR} \geq \mathrm{LLR}_{\mathrm{obs}} \mid \mathrm{b}\right)$, with $P$ representing the conditional probabilities. $\mathrm{CL}_{\mathrm{s}}$ is then defined as $\mathrm{CL}_{\mathrm{s}}=\mathrm{CL}_{\mathrm{s}+\mathrm{b}} / \mathrm{CL}_{\mathrm{b}}$. By repeating implementations of the procedure described in Section 5, for each mass point, the CL in the signal $\left(\mathrm{CL}_{\mathrm{s}}\right)$ as a function of a cross-section scaling factor $\mu$ was obtained keeping the mass window fixed. A scan is performed over a range of $\mu$ until one crosses the $\mathrm{CL}_{\mathrm{s}}=0.05$ value.

The scaling factor $\mu$ for a $95 \%$ CL exclusion was calculated by a linear interpolation between these points and then converted into an upper limit. For a given mass, a re-scaling of the cross-section would imply a change in the width of the resonance. Thus, for each mass point, the available signal template with the $k / \bar{M}_{\mathrm{Pl}}$ value closest to the expected $95 \%$ limit was chosen. This way, the change in the shape was minimized.

Figure 6 shows the $95 \%$ CL limits on the production cross section times branching ratio of an RS model graviton decaying into two photons as a function of the lightest graviton mass. Superimposed are the theoretical cross section predictions for a variety of $k / \bar{M}_{\mathrm{Pl}}$ values with the bands representing the uncertainty on the cross sections as described in section 6 . The results are interpreted in the $k / \bar{M}_{\mathrm{Pl}}$ versus graviton mass plane in Fig. 7 and compared to the Tevatron results.


Figure 6: The $95 \% \mathrm{CL}$ on the production cross section times branching ratio of an RS model graviton decaying into two photons $(\sigma \times \operatorname{Br}(G \rightarrow \gamma \gamma))$ as a function of the graviton mass. Superimposed are the theoretical cross section prediction bands for a variety of $k / \bar{M}_{\mathrm{Pl}}$ values.


Figure 7: $95 \%$ CL excluded region in the plane of $k / \bar{M}_{\mathrm{Pl}}$ versus graviton mass. Also shown are the expected limit and published limits from the Tevatron experiments [3] [4].

## 8 Summary

No evidence of a narrow resonance decaying into a pair of photons above the continuum background is observed. The results are used to set limits on the production of Randall-Sundrum gravitons decaying into diphoton final states. The results exclude at 95\% CL RS graviton masses below 545 (920) GeV for the dimensionless RS coupling $k / \bar{M}_{\mathrm{Pl}}=0.02(0.1)$.

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## Data-driven estimation of the background to charged Higgs boson searches using hadronically-decaying $\tau$ final states in ATLAS

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#### Abstract

The experimental observation of charged Higgs bosons, $H^{ \pm}$, which are theoretically predicted by many non-minimal Higgs scenarios, would indicate new physics beyond the Standard Model. In the Minimal Supersymmetric Standard Model, for example, the dominant production mode at the LHC for these Higgs bosons, when $m_{H^{+}}<m_{t}$, takes place in $t \bar{t}$ events via the top-quark decay $t \rightarrow H^{+} b$ with $H^{+} \rightarrow \tau v$ dominating for most values of $\tan \beta$. Two channels with a hadronically decaying $\tau$ coming from the charged Higgs boson are studied. The delivery of the first $37 \mathrm{pb}^{-1}$ of $\sqrt{s}=7 \mathrm{TeV}$ collision data allows many significant backgrounds to be estimated with data-driven methods, which represent the primary focus of this note and a crucial step towards ATLAS searches for the charged Higgs boson.


## 1 Introduction

The charged Higgs boson is predicted by many non-minimal Higgs scenarios such as models containing Higgs triplets and 2-Higgs-Doublet Models (2HDM) [1, 2, 3]. The experimental observation of charged Higgs bosons ${ }^{1}, H^{ \pm}$, would indicate new physics beyond the Standard Model. The first experimental evidence for the Minimal Supersymmetric Standard Model (MSSM) might very well come from their discovery at the Large Hadron Collider (LHC), if the model is realized in nature, and supersymmetric particles are heavy enough to evade detection [4]. The analyses in this note only consider the 2HDM, more specifically the Type II-2HDM, which describes the Higgs sector of the MSSM.

The dominant production mode at the LHC for these Higgs bosons for the case that the charged Higgs boson mass ( $m_{H^{+}}$) is smaller than the top-quark mass $\left(m_{t}\right)$ are $t \bar{t}$ events via the top-quark decay $t \rightarrow H^{+} b$ with $H^{+} \rightarrow \tau v$ (see Figure 1). The $H^{+} \rightarrow \tau v$ decay mode dominates if the ratio of the vacuum expectation values of the two Higgs doublets $(\tan \beta)$ is larger than 3. Production in the $\tau+\mathrm{jets}$ channel occurs when one of the two top quarks decays to $W b \rightarrow j j b$. Similarly, signal events considered by the $\tau+$ lepton channel come about when one of the top quarks decays to $W b \rightarrow l v b$ ( $l=e, \mu$ or leptonically decaying $\tau$ ). Both channels are studied here, but this note only considers a hadronically-decaying $\tau$ coming from the charged Higgs boson.

The background processes that enter these searches include the production of $t \bar{t}$, single top-quark, $W+$ jets, $Z+$ jets, and QCD multi-jet events. The delivery of the first collision data with a centre-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ allows many significant backgrounds to be estimated in a data-driven way, a crucial step toward searches for these bosons in the near future using ATLAS datasets with larger integrated luminosity. The methods used for background estimation are based on embedding $\tau$ jets in events with muons, and on the measured probabilities for jets, electrons, and muons to be misidentified as $\tau$ jets. Finally, the QCD multi-jet background is estimated in the $\tau+$ jets analysis using a data-driven control sample. The studies are based on proton-proton collision data collected at the LHC at a centre-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ in 2010. Only data-taking runs where all detector systems were fully operational and stable beam conditions were fulfilled are used. The total investigated luminosity corresponds to up to $37 \mathrm{pb}^{-1}$ and depends slightly on the trigger streams used.


Figure 1: Leading-order Feynman diagram for the production of a charged Higgs boson through gluongluon fusion in $t \bar{t}$ decays.

## 2 Physics processes and cross sections

The Monte Carlo (MC) simulation of $t \bar{t}$ and single top-quark events from proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ is done with MC@NLO [5] using HERWIG [6] for hadronization and JIMMY [7] for the

[^60]underlying event. Overlap between $t \bar{t}$ and single top-quark final states is removed in these MC@NLO samples [8]. A $t \bar{t}$ production cross section of 164.6 pb [9] obtained from NLO+NNLL calculations [10] is used (both for Standard-Model-like $t \bar{t}$ and decays via $H^{+}$); the MC@NLO values are used for single top-quark production.

ALPGEN [11] is used for the generation of $W$ and $Z$ events with up to five additional partons, again together with HERWIG/JIMMY. The MLM matching scheme [12] is employed, with the jet $p_{T}$ and $\Delta R$ cuts set to 20 GeV and 0.7 , respectively. The ALPGEN cross sections are rescaled by a factor $1.20(W)$ and $1.25(Z)$ to match NNLO calculations [4]. The $b \bar{b}$ and $H^{+}$events are generated with PYTHIA [13], using TAUOLA [14] for $\tau$ lepton decays and PHOTOS [15] for photon radiation off charged leptons. Events hadronized by PYTHIA use the ATLAS MinBias Tune 1 [16], while HERWIG/JIMMY samples use the ATLAS Underlying Event Tune 1 [17]. The simulated events and cross sections used are summarized in Table 1. The expected number of events is given by the production cross section times the integrated luminosity, which is $37 \mathrm{pb}^{-1}$ for the lepton triggers, and $36 \mathrm{pb}^{-1}$ for the hadronically-decaying- $\tau$ plus $E_{\mathrm{T}}^{\text {miss }}$ trigger. All events are passed through a detailed ATLAS detector simulation [18] using GEANT4 [19] and reconstructed by the same algorithms as the data.

Table 1: Simulated events used in this study. The $W / Z+j e t s, t \bar{t}$, as well as the $s$ - and $t$-channel single top-quark events are only simulated for decays involving leptons ( $e, \mu$, or $\tau$ ), and the cross section given includes this branching ratio. NLO+NNLL calculations are used for $t \bar{t}$, NLO for single top-quark, NNLO for $W / Z+$ jets, and LO for $b \bar{b}$. The $b \bar{b}$ cross section is given for the phase space with at least one muon in the decay chain with $p_{T}>15 \mathrm{GeV}$. The $H^{+}$sample uses $m_{H^{+}}=130 \mathrm{GeV}$ and $\tan \beta=35$ as input.

| Process | Generator | Cross section [pb] |
| :--- | :--- | ---: |
| $t \bar{t}$ with $\geq 1 \ell$ | MC@NLO | 89.7 |
| single top-quark $(s, t, W t$ channel $)$ | MC@NLO | $21.4,1.41,14.6$ |
| $W \rightarrow \ell v+$ jets | ALPGEN | $3.1 \cdot 10^{4}$ |
| $Z \rightarrow \ell \ell+$ jets | ALPGEN | $3.2 \cdot 10^{3}$ |
| $b \bar{b}$ with $\mu$ filter | PYTHIAB | $7.4 \cdot 10^{4}$ |
| $t \bar{t} \rightarrow b H^{ \pm} b W$ with $H^{ \pm} \rightarrow \tau v$ | PYTHIA | 18.5 |

## 3 Object reconstruction

In this section, the common object reconstruction for the $\tau+$ jets and $\tau+$ lepton event selections are detailed. For data-driven background estimation methods based on fake rates, requirements on the tag objects are explained in the respective sections should they differ.

Event-level cleaning cuts For both the $H^{+}$event selection and the data-driven background estimates several general-purpose event quality requirements [20] are always applied. To further reject noncollision backgrounds, only events with a reconstructed primary vertex with at least five associated tracks are considered.

Jets Jets are reconstructed with the anti- $k_{T}$ algorithm [21, 22] with a size parameter value of 0.4 , using three-dimensional topological clusters as input [23, 24]. The electromagnetic calibration of the ATLAS calorimeters is converted to the hadronic scale by a calibration scheme depending on $p_{T}, \eta$ and the number of primary vertices in the event [25]. Jets are required to have $p_{T}>20 \mathrm{GeV}$ and $|\eta|<4.9$. While the standard ATLAS definition is $|\eta|<4.5$, a looser pseudorapidity cut is used in this work.
$\tau$ jets For the reconstruction of hadronically-decaying $\tau \mathrm{s}$, anti- $k_{T}$ jets in the calorimeter with $E_{T}>10$ GeV are used as seeds. Electron and muon vetoes are applied at this stage, and $p_{T}>20 \mathrm{GeV},|\eta|<$ 2.5 , and 1 or 3 associated tracks are required. Objects passing this selection are referred to as " $\tau$ jet candidates". Additionally, medium (tight) quality cuts on the $\tau$ log-likelihood identification are applied for 1 -track (multi-track) $\tau$ jet candidates [26], to discriminate $\tau$ jets from jets not initiated by $\tau$ leptons.
$b$ jets A secondary-vertex tagger with a nominal efficiency of about $50 \%$ is used to identify those jets containing $b$ quarks among all jets passing the reconstruction discussed above [27].

Electrons Electrons are reconstructed by matching energy depositions in clusters of electromagnetic calorimeter cells to a track in the inner tracking detector [28]. The shower-shape information is used to increase the quality of the electron identification. Candidates are required to have $p_{T}>20 \mathrm{GeV}$ (for lepton vetoes, this value is lowered to 10 GeV ), and to be in the pseudorapidity ranges $0<|\eta|<1.37$ or $1.52<|\eta|<2.47$. Only isolated electrons are considered by requiring that the deposited energy in a calorimeter cone of $\Delta R<0.2$ around the electron ${ }^{2}$ is less than 4 GeV plus $2.3 \%$ of the electron $E_{T}$.

Muons Objects are considered as muon candidates if an inner detector track matches a track reconstructed in the muon spectrometer [29]. Candidates are required to have $p_{T}>20 \mathrm{GeV}$ (for lepton vetoes, this value is lowered to 10 GeV ) and $|\eta|<2.5$. Only isolated muons are considered by requiring that in a cone of $\Delta R<0.3$ around the muon, both the energy deposited in the calorimeters and the momentum of all inner detector tracks total less than 4 GeV . Additionally, an angular distance to any jet with $E_{T}>20$ GeV of $\Delta R>0.4$ is required.

Missing transverse energy, transverse energy sum The missing transverse energy, $E_{\mathrm{T}}^{\mathrm{miss}}$, is based on the energy deposited in the calorimeter and the momentum of tracks identified as associated to muons. The contribution of the calorimeter cells is calibrated differently depending on the object to which they are associated. For all jets, the same hadronic calibration scheme as for jet reconstruction is used while electrons are calibrated at the electromagnetic scale [30].

The transverse energy sum, $\Sigma E_{\mathrm{T}}$, is defined as the sum of the transverse energy of all objects which have been reconstructed as detailed in this section, i.e., electrons, muons, $\tau$ jets, $b$-tagged jets, light jets, and $E_{\mathrm{T}}^{\mathrm{miss}}$.

The missing transverse energy significance, $E_{\mathrm{T}}^{\text {miss }} / \sqrt{\Sigma E_{T}}$, is a complex quantity used to suppress QCD multi-jet events without losing a large number of signal events (simply increasing the $E_{\mathrm{T}}^{\text {miss }}$ requirement would be detrimental to the $\tau+$ jets analysis). As discussed in Reference [31], investigations have shown that this quantity is well-modeled for events with a large amount of true $E_{\mathrm{T}}^{\mathrm{miss}}$.

Overlap removal When candidates selected using the above criteria overlap within $\Delta R<0.2$, this is resolved by calling the object a muon, electron, $\tau$ jet, or jet, in this order of priority.

### 3.1 Object-related systematic uncertainties

Uncertainties on the reconstruction and identification of leptons, $\tau$ jets and other jets, as well as the momentum or energy resolution/scale of these objects, comprise the dominant detector-related contributions to the systematic uncertainties. Additionally, uncertainties due to missing transverse energy reconstruction, the trigger, and measured luminosity are considered.

[^61]In lieu of a sizeable sample of true $\tau$ jets collected from collision data, the systematic uncertainty for the $\tau+E_{\mathrm{T}}^{\mathrm{miss}}$ trigger is estimated from the differences between simulation and data observed for this trigger in QCD multi-jet events. This results in a conservative estimate as the comparison is done on QCD multi-jet events rather than true $\tau$ jets-where the systematic effect is expected to be smaller. The statistical uncertainty on the ratio of the simulation-to-data trigger efficiencies (which is compatible with 1), in a region of transverse energy that benefits from large statistics, is taken as the systematic uncertainty on the $\tau$ trigger efficiency ( $11 \%$ ). For the $E_{\mathrm{T}}^{\text {miss }}$ trigger efficiency, the systematic uncertainty is taken as the largest simulation-to-data discrepancy observed for events with $E_{\mathrm{T}}^{\text {miss }}>50 \mathrm{GeV}$ (where the bulk of selected data lies) and is $5 \%$. The $\tau$ and $E_{\mathrm{T}}^{\text {miss }}$ trigger uncertainties are combined under the assumption that they are uncorrelated.

The dominating experimental systematic uncertainties for the $H^{+}$studies are summarized in Table 2. To assess the impact of most systematic sources on either the $\tau+$ jets or the $\tau+$ lepton channel, the selection cuts for each analysis are applied after shifting a particular parameter to its upper and lower extrema. The luminosity and the trigger uncertainty with respect to the offline efficiency both serve directly as scale factors on the event yield.

The effect of various systematic uncertainties on data-driven background estimates based on either $\tau$ jet fake rates, embedding, or the inversion of event selection criteria, some of which are unique to the methods themselves, is explored in Section 5.

Table 2: Object-related systematic uncertainties.

| Source of uncertainty | Uncertainty used in this analysis |
| :--- | :--- |
| Luminosity | $\pm 11 \%$ |
| $E_{\mathrm{T}}^{\text {miss }}$ resolution | Add or subtract object uncertainties into the $E_{\mathrm{T}}^{\text {miss }}$, up to $\pm 20 \%$ |
| Jet energy resolution (JER) | $\approx \pm 14 \%$, depending on $\eta$, see Reference [32] |
| Jet energy scale (JES) | $< \pm 10 \%$ for $p_{\mathrm{T}}>15 \mathrm{GeV}$ and $\|\eta\|<4.5$, see Reference [33] |
| b-tagging efficiency | $p_{\mathrm{T}}$ dependent scale factor uncertainties, $\pm 10-12 \%$, see Reference [27] |
| b-tagging mistag rate | Up to $\pm 26 \%$, Reference [27] with further refinements |
| Tau identification efficiency | $\pm 6-12 \%$, depending on $p_{\mathrm{T}}$ and number of associated tracks |
| Tau energy scale | $\pm 5 \%$ |
| Electron selection efficiency | $\pm 6-16 \%$ as a function of $p_{\mathrm{T}}$ |
| Electron energy scale | $\pm 1 \%$ for $\eta \mid<1.4, \pm 3 \%$ for $1.4<\|\eta\|<2.5$ |
| Electron energy resolution | Sampling term $\pm 20 \%$, a small constant term has a large variation with $\eta$ |
| Muon selection efficiency | $\pm 1.2 \%$ for $p_{\mathrm{T}}<20 \mathrm{GeV}$ and $\pm 0.4 \%$ for $p_{\mathrm{T}}>20 \mathrm{GeV}$ |
| Muon momentum scale | $\eta$ dependent scale offset in $p_{\mathrm{T}}$, up to $\pm 3.5 \%$ |
| Muon momentum resolution | $p_{\mathrm{T}}$ and $\eta$ dependent resolution smearing functions, $\leq \pm 10 \%$ |
| $\tau+E_{\mathrm{T}}^{\text {miss }}$ trigger | $\pm 12 \%$ with respect to offline, References [34,35] with further refinements |

## 4 Event selection

### 4.1 Event selection in the $\tau+$ jets final state

A topology of interest in the search for a charged Higgs boson decaying to $\tau v$ is

$$
\begin{equation*}
t \bar{t} \rightarrow\left[H^{+} b\right]\left[W^{-} \bar{b}\right] \rightarrow\left[\left(\tau^{+} v\right) b\right][(j j) \bar{b}] \tag{1}
\end{equation*}
$$

where both the $W$ boson and the $\tau$ lepton decay hadronically; the neutrinos result in a large amount of $E_{\mathrm{T}}^{\mathrm{miss}}$. This topology has several advantages: the fact that the $W$ boson can be reconstructed fully; the $H^{+}$candidate mass can be reconstructed in the transverse plane (analogous to the transverse mass in
a $W$ decay); and the larger branching fraction for $W$ decaying into hadrons. However, there are also potentially serious challenges, such as the inherent presence of multi-jet final states which may make it difficult to distinguish this topology from the QCD multi-jet background.

The event selection is based on $E_{\mathrm{T}}^{\text {miss }}$ and $\tau$-trigger selection, followed by the offline selection involving jets, $b$ jet tagging, $\tau$ identification, and the selection of the highest- $p_{T} j j b$ candidate (i.e., the reconstructed top-quark candidate from the decay $t \rightarrow W b \rightarrow$ jet-jet-b). The baseline selection is based on the objects and definitions in Section 3 and consists of the following requirements:

1. Event preselection:
(a) event-level cleaning cuts as described in Reference [20], with further refinements;
(b) $E_{\mathrm{T}}^{\text {miss }}$ plus $\tau$-trigger;
(c) at least 4 jets with $p_{T}>20 \mathrm{GeV}$ and $|\eta|<4.9$.
2. Exactly one $\tau$ jet candidate with $p_{T}>20 \mathrm{GeV}$.
3. Events with any identified electrons or muons with $p_{T}>10 \mathrm{GeV}$ are vetoed.
4. $E_{\mathrm{T}}^{\mathrm{miss}}>20 \mathrm{GeV}$.
5. $E_{\mathrm{T}}^{\mathrm{miss}} / \sqrt{\Sigma E_{\mathrm{T}}}>3 \mathrm{GeV}^{1 / 2}$.
6. At least one $b$-tagged jet.
7. The $j j b$ system candidate with the highest $p_{T}^{j j b}$ value must satisfy $m(j j b) \in[120,240] \mathrm{GeV}$.

The final discriminating variable is the $\tau+E_{\mathrm{T}}^{\text {miss }}$ transverse mass, $m_{T}$, which in the case of most backgrounds corresponds to the transverse $W$ mass and in the case of the signal hypothesis corresponds to the transverse $H^{+}$mass. Explicitly, $m_{T}$ is defined as

$$
\begin{equation*}
m_{T}=\sqrt{2 p_{T}^{\tau} E_{\mathrm{T}}^{\mathrm{miss}}(1-\cos \Delta \phi)} \tag{2}
\end{equation*}
$$

where $\Delta \phi$ is the angle between the $\tau$ jet and the missing momentum in the transverse plane. Using this selection, a total of 33 events are observed in $36 \mathrm{pb}^{-1}$ of data.

### 4.2 Event selection in the $\tau+$ lepton final state

In this channel, the event signature is based on the leptonically decaying $W$ boson $(l=e, \mu$, or $\tau$ with $e / \mu$ decays) and the presence of a hadronically-decaying $\tau$. Neutrinos in the event result in a large amount of $E_{\mathrm{T}}^{\text {miss }}$

$$
\begin{equation*}
t \bar{t} \rightarrow\left[H^{+} b\right]\left[W^{-} \bar{b}\right] \rightarrow\left[\left(\tau^{+} v\right) b\right]\left[\left(l^{-} \bar{v}\right) \bar{b}\right] \tag{3}
\end{equation*}
$$

The signal can manifest itself as an excess of $\tau$ leptons above the irreducible Standard Model background of $t \bar{t}$ production. Since at least three neutrinos are expected to be present in the final state, a full event reconstruction is not possible. The lepton originating from the $W$ decay allows for the use of a highly efficient trigger.

The baseline event selection is built around an isolated lepton trigger requirement, missing transverse energy, tagged $b$ jets, and a $\tau$ jet. It is based on the objects and definitions in Section 3 and consists of the following requirements:

1. Event preselection:
(a) event-level cleaning cuts as described in Reference [20], with further refinements;
(b) lepton trigger;
(c) exactly one trigger-matched isolated lepton with $p_{T}>20 \mathrm{GeV}$.
2. Exactly one $\tau$ jet with $p_{T}>20 \mathrm{GeV}$.
3. At least two jets with $p_{T}>20 \mathrm{GeV}$ and $|\eta|<4.9$.
4. At least one of the jets is $b$-tagged.
5. $\sum E_{\mathrm{T}}>200 \mathrm{GeV}$.
6. Selected $\tau$ jet and lepton have opposite charge.
7. $E_{\mathrm{T}}^{\text {miss }}>60 \mathrm{GeV}$.

Using this selection, a total of 11 events are observed in $37 \mathrm{pb}^{-1}$ of data.

## 5 Data-driven background estimation

Events coming from production processes such as $t \bar{t}$, single top-quark, $W+$ jets, $Z+$ jets and QCD multijets make up the dominant background to charged Higgs boson searches at the LHC. The individual contributions from many of these backgrounds can be determined in a data-driven way. Events in which electrons, muons, or jets are misidentified as $\tau$ jets are predicted using methods based on fake rates. In this note, a fake rate is understood as the number of objects ( $e, \mu$ or jet) being identified as a $\tau$ jet divided by all objects considered for $\tau$ identification (called $\tau$ jet candidates). Background events containing true $\tau$ jets are studied with the embedding method. The QCD multi-jet background is estimated in the $\tau+$ jets analysis using a data-driven control sample.

### 5.1 Events with electrons misidentified as $\tau$ jets

The $\tau$ identification has been optimized separately for a high QCD jet rejection, and for the rejection of electrons [26]. The probability that an electron is misidentified as a $\tau$ jet can be estimated from data.

### 5.1.1 Method

A technique to derive this fake rate from data is the so-called tag-and-probe method. The process $Z \rightarrow e e$ allows the selection of an unbiased and clean sample of electrons from data. While the tag electron is required to satisfy a tight electron selection, the other, if it is reconstructed as a $\tau$ jet candidate, is then used as the probe.

Only those probe $\tau$ jet candidates with exactly one associated track are considered as the rate of electrons faking 3 -track $\tau$ jets is negligible compare to the 1 -track case. The individual requirements for both the $\tau+$ jets and $\tau+$ lepton analyses are applied, this includes the electron veto and the overlap removal with electron candidates.

### 5.1.2 Results

The measured fake rates are shown in Figure 2. Within uncertainties, the fake rates modeled in Monte Carlo agree with those obtained from data.

### 5.1.3 Systematic uncertainties

Three main sources of systematic uncertainties on the electron-to- $\tau$ fake rate have been studied. The largest contribution originates from the background contamination with QCD jets (after the application of the electron veto on the probe object, QCD jets are enhanced with respect to electrons among the $\tau$ jet candidates) and gives an uncertainty of about $30 \%$. The choice of the mass window size around the $Z$ boson mass applied to the tag-and-probe objects introduces another uncertainty ( $13 \%$ ). The uncertainty of the electron energy scale (via the cut on the tag electron energy) only gives a small contribution (2\%). The total systematic uncertainty varies slighty with $p_{\mathrm{T}}$ and $\eta$ and is estimated to be $33 \%$.


Figure 2: The fake rate for probe objects passing the $\tau$ identification, the electron veto, and overlap removal with reconstructed electrons is shown parametrized in $p_{T}$ and $|\eta|$. The uncertainties indicated are statistical only.

### 5.1.4 Application to estimate the electron-to- $\tau$ fake background to the $H^{+}$selections

The electron-to- $\tau$ fake background is estimated the following way: In simulated events, any true electron matched to a $\tau$ jet candidate is labeled as an identified $\tau$ jet and the event is given a weight equal to the probability given by the fake rate measured in this section, instead of performing the usual $\tau$ identification (i.e. the $\tau$ identification part is taken from data instead of simulation). All relevant quantities ( $E_{\mathrm{T}}^{\mathrm{miss}}, \Sigma E_{T}$, $E_{\mathrm{T}}^{\mathrm{miss}}$ significance, $m_{T}$, opposite-charge requirement) are then recalculated under the hypothesis that the electron is identified as a $\tau$ jet. The baseline selections of both the $\tau+$ jets and the $\tau+$ lepton channels (with the exception of the $\tau$ log-likelihood identification requirements) are then applied and the number of events surviving is counted (summing the weights of these events). The prediction using the fake rate derived from data and the expectation from Monte Carlo are shown in Table 3.

Table 3: Application of the fake rate obtained from $Z \rightarrow e e$ events. The numbers shown are the expected number of events after the baseline $\tau+$ lepton selection (normalized to $37 \mathrm{pb}^{-1}$ ), and after the baseline $\tau+$ jets selection (normalized to $36 \mathrm{pb}^{-1}$ ), for one-track $\tau$ jets. The predictions based on the fake rate measurement (the first uncertainty is statistical and the second is systematic), as well as the Monte Carlo prediction (statistical uncertainties only), are given.

| Selection | Sample | Fake rate prediction [num. of events] | MC prediction [num. of events] |
| :--- | :--- | :--- | :--- |
| $\tau+$ jets | $t \bar{t}$ | $1.08 \pm 0.01$ (stat) $\pm 0.38$ (syst) | $1.50 \pm 0.09$ (stat) |
| $\tau+$ lepton | $t \bar{t}$ | $0.65 \pm 0.01$ (stat) $\pm 0.04$ (syst) | $0.79 \pm 0.08$ (stat) |

### 5.2 Events with muons misidentified as $\tau$ jets

The muon-to- $\tau$ fake rate has been studied in a control sample of $Z \rightarrow \mu \mu$ events, in a similar manner as the electron-to- $\tau$ fake rate described in Section 5.1. The Monte Carlo description of the muon-to- $\tau$ fake rate is found to be consistent with that in data. Since the Monte Carlo expectation is that this background is 2-3 orders of magnitude smaller than even the uncertainties of other backgrounds, it is concluded that the background due to muons misidentified as $\tau$ jets is negligible.


Figure 3: Jet-to- $\tau$ fake rates measured from $\gamma+$ jet events for 1 -track and 3-track $\tau$ jets. Statistical and systematic uncertainties are given for Monte Carlo, while the uncertainties shown for data are only statistical.

### 5.3 Events with jets misidentified as $\tau$ jets

A measurement of the probability of jets to be misidentified as $\tau$ jets is performed using $\gamma+\mathrm{jet}$ events selected from collision data. This particular control sample is selected as the jet in these events is dominantly quark-initiated (as opposed to QCD jets events, where jets are dominantly gluon-initiated) which is also the case for the background investigated in this section, i.e., $t \bar{t}$, single top-quark, and $W+$ jets. The resulting fake rate is used to predict the part of these backgrounds which is due to jet-to- $\tau$ fakes, for both the $\tau+$ jets and $\tau+$ lepton analyses.

### 5.3.1 Method

For the measurement of the jet $\rightarrow \tau$ fake rate, events are required to pass a $\gamma$ trigger. Identified $\gamma \mathrm{s}$ are required to be matched to the trigger object and pass a tight isolated photon selection. They must have $|\eta|<2.5$ and a transverse momentum of at least 25 GeV . Events are selected which have one $\gamma$ and a jet of $p_{\mathrm{T}}>20 \mathrm{GeV}$ separated by a $\Delta R$ of at least 0.7 . The fake rate is binned in number of tracks associated to the $\tau$ jet candidate and in $p_{\mathrm{T}}$. The object going into the denominator of the fake rate calculation is a $\tau$ jet candidate which must have $p_{\mathrm{T}}>20 \mathrm{GeV},|\eta|<2.5$, 1 or 3 associated tracks, and pass lepton vetoes in order to reduce lepton fakes that would otherwise contaminate the fake measurement.

Objects going into the numerator of the fake rate calculation must pass the complete $\tau$ identification as described in Section 3. They must also have between 1 and 3 associated tracks, not be within $\Delta R$ of 0.4 of any $e$ or $\mu$ passing the common object selection, and pass the cuts for reconstructed $\tau$ identification. Once measured, the fake rate can be applied to MC to test its ability to accurately measure the number of fakes and to predict fakes in data. The resulting fake rates are shown in Figure 3.

### 5.3.2 Systematic uncertainties

The systematic uncertainties considered are (the values depend slightly on $p_{T}$ ):

- Contamination of the control sample with true $\tau$ jets from $Z \rightarrow \tau \tau$ and $W \rightarrow \tau v$ (negligible).
- Contamination of the control sample with QCD multi-jet events. This is tested by investigating the effect of modifying the photon identification requirements on the measured fake rate, in particular loosening the photon isolation which increases the impurity from QCD jets in the control sample ( $\approx 10 \%$ ).
- Uncertainties of the control samples selection. This is tested by varying the selection cuts, and by splitting the control sample into a part which fulfils even tighter requirements and one which does not, and then taking the variation of the fake rate due to these changes as the uncertainty ( $\approx 15 \%$ ).
- Correlations between the tag and probe objects. This is evaluated by changing the selection requirements for the tag object and studying the impact on the fake rate $(\approx 3 \%)$.

The total systematic uncertainty is about $20 \%$ in the $p_{T}$ range of interest. The statistical uncertainty on the fake rate is a systematic uncertainty for any application of the fake rate, and grows rapidly with $p_{T}$, as shown in Figure 3.

### 5.3.3 Application to estimate the fake-jets background to the $H^{+}$selections

In simulated events, any jet matched to a $\tau$ jet candidate as defined by the denominator requirements of the fake rate detailed in Section 5.3 .1 is labeled as a $\tau$ jet (instead of performing the offline hadronic $\tau$ identification), and given a weight equal to the calculated fake rate value. In order to avoid doublecounting, the jet that corresponds to this hadronic $\tau$ is removed from the event, affecting the number of reconstructed jets, $\Sigma E_{T}$ of the event, $E_{\mathrm{T}}^{\text {miss }}$, the $E_{\mathrm{T}}^{\text {miss }}$ significance, the number of $b$-tagged jets, and the top quark reconstruction. For all events which pass the event selection after taking this into consideration, the weight is summed. The number of events predicted for collision data, together with a comparison to the prediction using Monte Carlo truth information, is shown in Table 4 both for the $\tau+$ jets and the $\tau+$ lepton baseline selection (see Section 4). Within uncertainties, the predictions agree well.

Table 4: Application of the fake rate obtained from $\gamma+$ jet events. The numbers shown are the expected number of events in collision data after the baseline $\tau+$ lepton selection (normalized to $37 \mathrm{pb}^{-1}$ ), and after the baseline $\tau+$ jets selection (normalized to $36 \mathrm{pb}^{-1}$ ). The predictions based on the fake rate measurement (statistical and systematic uncertainties), as well as the Monte Carlo prediction (statistical uncertainties), are given.

| Selection | Sample | Fake rate prediction [num. of events] | MC prediction [num. of events] |
| :--- | :--- | :--- | :--- |
| $\tau+$ jets | $t \bar{t}$ | $1.7 \pm 0.2$ (stat) $\pm 0.3$ (syst) | $1.9 \pm 0.2$ (stat) |
| $\tau+$ lepton | $t \bar{t}$ | $6.7 \pm 1.0$ (stat) $\pm 1.4$ (syst) | $6.0 \pm 0.2$ (stat) |
| $\tau+$ lepton | $W+$ jets | $0.9 \pm 0.1$ (stat) $\pm 0.2$ (syst) | $0.6 \pm 0.3$ (stat) |
| $\tau+$ lepton | Single top | $0.16 \pm 0.02$ (stat) $\pm 0.03$ (syst) | $0.12 \pm 0.02$ (stat) |
| $\tau+$ lepton | $Z+$ jets | $0.15 \pm 0.02$ (stat) $\pm 0.03$ (syst) | $0.3 \pm 0.2$ (stat) |

### 5.4 QCD Background Estimate

### 5.4.1 Method

The following method is used to estimate the QCD jets background to the $\tau+\mathrm{jets}$ analysis. In order to model the QCD background from data, an orthogonal event selection is defined which is identical to the complete $\tau+$ jets event selection, except for requiring a looser $\tau$ identification while rejecting events using the tighter $\tau$ identification used in the baseline selection.

This selection, referred to as "inverted selection" in this section, is applied to data and the shape of the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution is used as a model for the QCD background (after subtracting the contribution from the background expectation from simulation for non-QCD processes). Then, a fit is performed to the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution in data resulting from the baseline $\tau+$ jets selection (after all cuts), using two shapes:
the model extracted for the QCD background, and the sum of non-QCD processes (dominated by $t \bar{t}$, $W+$ jets) for which the shape and the relative normalization is taken from MC simulation.

The fit floats the overall normalization (to the one in data) and the QCD fraction. The underlying assumption is that the shape of the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution for QCD is the same for the baseline and the inverted selection. This is shown in Figure 4 where the two distributions are compared for collision data. The comparison is done after selection cuts $1-3$ as described in Section 4.1 have been applied, as this ensures that the distributions are QCD-dominated. In spite of the QCD-dominance, the contribution of events with true $E_{\mathrm{T}}^{\text {miss }}$, like $t \bar{t}$ and $W+$ jets, is still significant in the tail of the distribution. For this reason, their expectation from simulation has been subtracted. Only a very small number of QCD events is observed for $E_{\mathrm{T}}^{\text {miss }}>100 \mathrm{GeV}$, as expected. The remaining differences are within statistical uncertainties.


Figure 4: Distribution of $E_{\mathrm{T}}^{\text {miss }}$ for data, after subtracting the expectation from $t \bar{t}, W+\mathrm{jets}$ and single topquark simulation. The comparison is done after selection cuts 1-3 as described in Section 4.1 have been applied, as this ensures that the distributions are QCD-dominated. The error bars show the size of the data statistical uncertainties.

### 5.4.2 Results

The result of the fit is shown in Figure 5. The QCD fraction is estimated to be ( $54 \pm 19$ ) \% for the 1-track $\tau$ case. There are not enough 3-track events in data after the baseline selection, thus no separate fit is performed and instead, both the 1- and 3-track cases are fitted simultaneously. The QCD fraction is estimated to be $(57 \pm 19) \%$.

### 5.4.3 Systematic uncertainties

The dominant systematic uncertainties are:

- Using $t \bar{t}$ and $W+$ jets shape and relative normalization from Monte Carlo, dominated by uncertainties on the $t \bar{t}$ cross section: $15 \%$.
- $E_{\mathrm{T}}^{\text {miss }}$ shape difference in signal and control region: $5 \%$.

The contamination in the control region from backgrounds that were not considered is negligible. Currently, the systematic uncertainty is dominated by the statistical uncertainty of the limited size of the data set on which the fit is applied, amounting to $33 \%$. However, this component will naturally decrease as the collected integrated luminosity increases. Uncertainties related to the cross sections and shapes of other backgrounds will also decrease once they are measured with high accuracy at the LHC.


Figure 5: Fit to $E_{T}^{\text {miss }}$ after all selection cuts using two shapes: one for the QCD model and one for $t \bar{t}$ and $W+$ jets (all other backgrounds are negligible and not shown). Left: 1 -track $\tau$ jets. Right: 1 -track and 3 -track $\tau$ jets together. The error bars show the size of the data statistical uncertainties.

### 5.4.4 Application to estimate the QCD background to the $\tau+$ jets selection

The estimated QCD jets contribution to the final $m_{T}$ distribution is shown in Figure 6. All other backgrounds have $W$ bosons in the final state and their distributions drop off around the $W$ boson mass, as expected. Such behaviour is neither expected nor observed for the QCD jets background as the sources of both the $\tau$ jet and $E_{\mathrm{T}}^{\text {miss }}$ are fakes and the resulting shapes are thus not steered by a specific physics process but by instrumental effects. To probe the region with large $m_{T}$, in which a potential $H^{+}$signal resides, it is thus important to suppress the QCD jets background as much as possible. This can be done with a tighter $\tau$ identification and harder $E_{\mathrm{T}}^{\text {miss }}$ requirements once a larger data set becomes available. The estimated QCD jets contribution after all cuts is $18.8 \pm 6.2$ (stat) $\pm 3.0$ (syst) events.


Figure 6: Estimated QCD jets contribution to the $m_{T}$ distribution after all cuts of the baseline $\tau+$ jets selection. The data is shown, together with the fit for $t \bar{t}$ and $W+$ jets contributions, where the shapes have been taken from simulation. The error bars show the size of the data statistical uncertainties.

### 5.5 Embedding method

Embedding tools are used for estimating the background with true $\tau$ jets for the $\tau+$ jets analysis. The method consists of collecting a control sample containing $t \bar{t}$, single top-quark production and $W+$ jet events with muons, replacing the detector signature of the muon with a simulated $\tau$ lepton, re-reconstructing the new hybrid event, and then using these events instead of simulation for background estimation. The advantage is that the whole event (except for the $\tau$ jet) is taken directly from data, including the underlying event and pile-up, $b$-quark jets and light-quark jets.

### 5.5.1 Method

Control sample collection. To select the $\mu+$ jets control sample from data, the following event selection is used, based on the objects and definitions in Section 3:

- Event-level cleaning cuts.
- Event passed a trigger requiring the presence of a muon candidate.
- Exactly one isolated muon with $p_{T}>20 \mathrm{GeV}$.
- No electron with $p_{T}>20 \mathrm{GeV}$.
- At least three jets with $p_{T}>20 \mathrm{GeV}$.
- At least one of the jets is tagged as $b$ jet.
- A reconstructed invariant mass of two jets with $p_{T}>35 \mathrm{GeV}$ in a mass window of 20 GeV around the nominal $W$ boson mass.
- Missing transverse energy $E_{T}^{\text {miss }}>30 \mathrm{GeV}$.
- Scalar sum of the energy in the calorimeter $\Sigma E_{T}>200 \mathrm{GeV}$.

The expected and observed number of events are shown in Table 5 and agree well.
Table 5: Expected (from simulation) and observed number of events in the embedding control sample. Statistical uncertainties only.

|  | Expected |  |  |  |  | Observed |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | $t \bar{t}$ | Single top-quark | $W+$ jets | QCD | Sum | Data |
| Events | $171.2 \pm 1.4$ | $11.3 \pm 0.3$ | $16.8 \pm 2.1$ | $12.4 \pm 3.2$ | $212 \pm 7$ | 219 |

The impurity from backgrounds with muons produced in $\tau$ decays, and non-isolated muons (dominantly $b \bar{b}$ and $c \bar{c}$ events) is at the level of $10 \%$ and biases the shape of embedded events as there is no physical correspondence to such embedded events. However, as is shown below, the bias is reduced as these events typically have a softer $\mu$ spectrum ( $W \rightarrow \tau \nu \rightarrow \mu \nu \nu \nu$ as compared to $W \rightarrow \mu \nu$, and muons from $B$ and $D$ meson decays) and thus mostly contribute to the low-mass tail of the $m_{T}$ distribution which is not considered.

Embedding step. After events have been selected, the actual embedding takes place. The muon in the event is selected, its vertex position and momentum are extracted. The momentum is then rescaled to account for the higher $\tau$-lepton mass, and fed into TAUOLA to produce the $\tau$-lepton decay products and generate final-state radiation. The result is propagated through the ATLAS detector simulation, followed by reconstruction.

In the next step, tracks and calorimeter cell depositions in the vicinity of the muon are replaced with those of the $\tau$-lepton decay products-in other words, the simulated $\tau$ event is embedded in the collision data event. Then the reconstruction algorithms are re-run on this hybrid event, reconstructing $\tau$ jets, leptons, missing transverse energy, and other high-level physics objects.

### 5.5.2 Application to estimate the true- $\tau$ background to the $\tau+$ jets selection

The contribution of backgrounds with true $\tau$ jets to the final $m_{T}$ distribution is estimated from this distribution for embedded events. The normalization is taken from collision data events in the region $30<m_{T}<70 \mathrm{GeV}$, where both the QCD background contribution and the signal contamination are low. The following procedure is applied:

1. Obtain the $m_{T}$ distribution after the $\tau+\mathrm{j}$ ets baseline selection from embedded events.
2. From collision data, count the number of events after applying the $\tau+$ jets selection in the $m_{T}$ distribution between $30<m_{T}<70 \mathrm{GeV}$ (after subtracting the background from fake $\tau$ jets).
3. Using this number, normalize the $m_{T}$ distribution from embedding using the ratio of events in collision data and embedded events in the region $30<m_{T}<70 \mathrm{GeV}$.

Currently, the method is statistics-limited and thus the selection applied to the embedded events is loosened compared to that given in Section 4.1: no trigger requirement is applied to the embedded samples and the $\tau$ identification is replaced by matching a $\tau$ candidate to the true $\tau$ in the event. Requirements related to the second top quark $t \rightarrow b q q$ in the event are dropped as they are not expected to influence the $m_{T}$ shape, namely the reconstruction of this hadronic top quark in a mass window and the requirement of having at least four jets in the event (loosened to three). In Figure 7, it is shown that the impact of this loosened selection on the $m_{T}$ shape, as compared to the same distribution for the baseline selection, can be taken into account by a systematic uncertainty of $20 \%$, which is less than the statistical uncertainty associated to the set of embedding events. Figure 7 also shows the $m_{T}$ distribution obtained from embedded simulation events (left) and data (right).


Figure 7: Left: Comparison of the $m_{T}$ shape in simulation for selections which have been loosened with respect to the $\tau+$ jets selection. Shown is the shape for the full selection (Baseline), and when removing the trigger, the $\tau$ identification requirement (replaced by matching a $\tau$ candidate to a true $\tau$ ), not using the top quark reconstruction requirement and only requiring a minimum of three instead of four jets (Loose). Additionally, this loosened selection is also applied to an embedded $t \bar{t}$ simulation sample (Embedded). Statistical uncertainties are shown. Right: Comparison of the $m_{T}$ shape embedded versus collision data after subtracting the contributions from fake $\tau$, as estimated in previous sections, from the data. The comparison is done after the $\tau+$ jets event selection described in Section 4.1 and after normalizing the embedding distribution to the data distribution in the range $30<m_{T}<70 \mathrm{GeV}$. Statistical and systematic uncertainties are shown.

As can be seen, the background estimate is currently limited by the statistical uncertainty due to the limited number of events in the $t \bar{t}$ control sample. In the range $70<m_{T}<210 \mathrm{GeV}, 4.7 \pm 1.3_{-1.1}^{+1.4}$ background events with true $\tau$ jets are expected and $6.3 \pm 2.5$ are observed in excess of the background predicted by the fake rate methods and the QCD fit. Within large statistical uncertainties, the background prediction and data agree well.

### 5.5.3 Systematic uncertainties

The following systematic uncertainties are associated to the background prediction:

- Differences in shapes of distributions between events with an embedded $\tau$ compared to a reference; considering Figure 7, the uncertainy is estimated to be $\pm 10 \%$. This includes the impact of the control sample selection (e.g. the muon trigger efficiency, the $\eta$ dependence of the offline muon selection) and the contamination from non-isolated muons and muons from $\tau$ decays.
- Difference in $m_{T}$ shape due to the loosening of the selection with respect to the baseline selection, as shown in Figure 7: $-20 \%$.
- Uncertainties in the subtraction of fake- $\tau$ backgrounds from data: $\pm 20 \%$.

An additional statistical uncertainty of about $30 \%$ is larger than the systematic uncertainties.

## 6 Summary of data-driven estimates

The results of the data-driven methods introduced and explained in Section 5 are summarized for each of the $\tau+$ jets and $\tau+$ lepton final state analyses, and compared to collision data.

## $6.1 \quad \tau+$ jets channel

The results of the data-driven methods in estimating the contributions of the various categories of backgrounds after the baseline selection are summarized in Table 6 and the $m_{T}$ distribution of the remaining events is shown in Figure 8. The number of events with true $\tau$ jets has been estimated with the embedding method, the jet $\rightarrow \tau$ fakes with $\gamma+$ jet control samples, the $e \rightarrow \tau$ fakes with $Z \rightarrow e e$ control samples and the QCD contribution by taking its shape from a sideband region and fitting it to the data. Both the total number of events, and the number of events with $m_{T}>70 \mathrm{GeV}$ is given. This allows for a better comparison of data and expectation as the estimate from the embedding method is fitted to data in the range $30<m_{T}<70 \mathrm{GeV}$. The uncertainties are still large, but a good agreement between estimated and observed events is seen.

Table 6: Expected number of events from data-driven estimates and as observed in data for the $\tau+$ jets channel.

|  | Expected |  |  |  | Observed |  |
| :--- | ---: | :---: | :---: | :---: | :---: | :---: |
|  | True $\tau$ jets | Jet $\rightarrow \tau$ fakes | $e \rightarrow \tau$ fakes | QCD | Sum | Data |
| All events | $10.8 \pm 3.1_{-2.4}^{+3.2}$ | $1.7 \pm 0.2 \pm 0.3$ | $1.1 \pm 0.0 \pm 0.4$ | $18.8 \pm 6.2 \pm 3.0$ | $32 \pm 9 \pm 7$ | 33 |
| $m_{T}>70 \mathrm{GeV}$ | $4.7 \pm 1.3_{-1.1}^{+1.4}$ | $1.2 \pm 0.2 \pm 0.2$ | $0.7 \pm 0.0 \pm 0.3$ | $11.3 \pm 3.7 \pm 1.7$ | $18 \pm 5 \pm 4$ | 17 |



Figure 8: The $\tau+E_{\mathrm{T}}^{\text {miss }}$ transverse mass distribution at the end of the event selection for the $\tau+\mathrm{jets}$ channel comparing the observation in collision data, and the estimates from data-driven methods. The error bars show the size of the data statistical uncertainties. The distribution of the $H^{+}$signal is given for a reference point in parameter space corresponding to $\mathrm{BR}\left(t \rightarrow b H^{+}\right) \approx 6 \%$, thus the SM-like $t \bar{t}$ background and its contribution to the $e \rightarrow \tau$ and jet $\rightarrow \tau$ fake background would be reduced correspondingly.

## $6.2 \tau+$ lepton channel

For the second final state under investigation, the results are summarized in Table 7 , and the $E_{\mathrm{T}}^{\text {miss }}$ distribution of the remaining events is shown in Figure 9. The number of events with true $\tau$ jets is taken from simulation, while the contribution of jet $\rightarrow \tau$ fakes and $e \rightarrow \tau$ fakes is estimated using $\gamma+\mathrm{jet}$ and $Z \rightarrow e e$ control samples. In this channel, the QCD jets background is negligible mostly due to the lepton and the $E_{\mathrm{T}}^{\mathrm{miss}}$ requirements. A good agreement between the estimated and the observed value is seen.

Table 7: Expected number of events from data-driven estimates and as observed in data for the $\tau+$ lepton channel. The number of events with true $\tau$ jets is taken from simulation.

|  | Expected |  |  |  | Observed |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | True $\tau$ jets | Jet $\rightarrow \tau$ fakes | $e \rightarrow \tau$ fakes | Sum | Data |
| Events | $6.9 \pm 0.3 \pm 1.4$ | $7.9 \pm 1.1 \pm 1.6$ | $0.65 \pm 0.01 \pm 0.04$ | $15.5 \pm 1.4 \pm 3.0$ | 11 |

## 7 Conclusions

Data-driven methods are used in $37 \mathrm{pb}^{-1}$ of $\sqrt{s}=7 \mathrm{TeV}$ data to estimate the number of events characterized by the presence of a $\tau$ jet, $E_{\mathrm{T}}^{\text {miss }}, b$ jets, and a hadronically or leptonically decaying $W$ boson. The events are predominantly expected to come from $t \bar{t}, W$ or $Z+$ jets, single top-quark, and QCD events and represent backgrounds to charged Higgs boson searches. Predictions of $32 \pm 9$ (stat) $\pm 7$ (syst)


Figure 9: The $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution at the end of the event selection for the $\tau+$ lepton channel comparing the observation in collision data, and the estimates from data-driven methods. The error bars show the size of the data statistical uncertainties. The distribution of the $H^{+}$signal is given for a reference point in parameter space corresponding to $\operatorname{BR}\left(t \rightarrow b H^{+}\right) \approx 6 \%$, thus the SM-like $t \bar{t}$ background and its contribution to the $e \rightarrow \tau$ and jet $\rightarrow \tau$ fake background would be reduced correspondingly.
$\left(18 \pm 5(\right.$ stat $) \pm 4$ (syst) with $\left.m_{T}>70 \mathrm{GeV}\right)$ and $15.5 \pm 1.4$ (stat) $\pm 3.0$ (syst) events are achieved in the $\tau+$ jets and $\tau+$ lepton channels, respectively. The observation of 33 events ( 17 with $m_{T}>70 \mathrm{GeV}$ ) in the $\tau+$ jets channel and 11 events in the $\tau+$ lepton channel is consistent with expectations based on these data-driven background estimation methods. The study presented here serves as a foundation for future charged Higgs boson searches in the hadronically-decaying $\tau$ final state using larger amounts of integrated luminosity.

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ATLAS NOTE
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# Update of Background Studies in the Search for the Higgs Boson in the Diphoton Channel with the ATLAS detector at $\sqrt{s}=7 \mathrm{TeV}$ 

The ATLAS collaboration


#### Abstract

This note presents an update of the study of the backgrounds in the search for the Higgs boson decaying into a pair of photons. The analysis done with $38 \mathrm{pb}^{-1}$ of $p p$ collision data collected in 2010 with the ATLAS detector at a centre-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ is complemented with $94 \mathrm{pb}^{-1}$ of data collected in 2011. The dominant background components are measured and found to be in agreement with the Standard Model predictions, both in terms of overall yield and invariant mass distribution. No excess is observed.


At this early stage of LHC operation an important question in the search for the Higgs boson in the diphoton decay channel is the relative contributions of the different background processes. The predominant background components are the irreducible prompt diphoton production, the reducible $\gamma$ jet and dijet backgrounds where one or more jets are misidentified as photons, and Drell-Yan events where both electrons are misidentified as photons. The measurement of these backgrounds is essential to accurately assess the performance of the search and to ascertain that all background processes are well modeled. This note presents an update of the study of backgrounds in the search for the Higgs boson in the $H \rightarrow \gamma \gamma$ channel, using a data sample corresponding to an integrated luminosity of $94 \mathrm{pb}^{-1}$ recorded in 2011 with the ATLAS detector at a centre-of-mass energy of 7 TeV . This luminosity estimate is based on a preliminary calibration; a $7 \%$ uncertainty is assigned in the normalization calculation. The computation of the expected backgrounds and the details of the data-driven background measurements follow closely the procedure described in [1, 2]. The two data sets of 2010 and 2011 are analyzed independently as the acceptance has changed due to the repair of faulty optical links in the calorimeter readout during the winter shutdown and because of the different running conditions.

Since the end of 2010 the LHC has been running with beams structured in bunch trains, with the number of bunches per train varying from 8 to more than 70 . The bunch spacing also varied from 150 ns in fall 2010 to 75 ns in March 2011 and down to 50 ns in April 2011. The changing beam patterns, in conjunction with the increasing beam intensities, have resulted in a variety of in-time and out-of-time pile-up conditions. An average number of interactions per bunch crossing of up to $\sim 8$ was reached. In this analysis a full Monte Carlo simulation, taking into account both the effects of in-time and out-oftime pile-up, was used. The efficiency of the photon identification and in particular that of the isolation cut are estimated using this simulation with high pile-up conditions.

The event selection is unchanged with respect to [1,2], except for the trigger thresholds where the transverse energy requirement for the two loosely selected photons has been raised from 15 GeV in 2010 to 20 GeV in 2011. Diphoton candidates are required to pass tight identification criteria, to be within the inner detector and calorimeter acceptance ( $|\eta|<2.37$ excluding $1.37<|\eta|<1.52$ ), to have transverse momenta larger than 40 GeV for the leading photon and 25 GeV for the sub-leading photon, and to have an invariant mass between 100 and 150 GeV . The photon isolation used in this analysis is calorimeter-based; it is corrected for underlying event and pile-up effects on an event-by-event basis, and for out-of-cone showering as described in [3]. Similarly to what was done in [1, 2] the Monte Carlo isolation efficiency is corrected for differences between the simulation and the data using electrons from $W$ decays collected in 2011.

The numbers of expected events for all background processes estimated for the 2011 running conditions are summarized in Table 1. The total expected background amounts to $301 \pm 72$ events. The main sources of uncertainties in these predictions are the jet fragmentation (into a photon or a leading $\pi^{0}$ ), the parton density functions and the variations of renormalization and factorization scales in the next-to-leading order predictions [1].

Altogether 291 diphoton candidate events are selected in the 2011 data, in good agreement with the overall Monte Carlo expectation. The number of prompt diphoton ( $N_{\gamma \gamma}$ ), photon-jet ( $N_{\gamma j}$ ) and dijet ( $N_{j j}$ ) events in the 2011 data sample are measured using the double sideband method described in [1, 2]. This method applies the sideband procedure of [3] to each photon sequentially. The sidebands are defined in terms of photon isolation and identification criteria using the fine-grained first sampling of the electromagnetic calorimeter. Since electrons from Drell-Yan events have a shower profile similar to that of isolated prompt photons, the $N_{\gamma \gamma}$ component estimated using the double sideband method contains most Drell-Yan dielectron events. The number of these events ( $N_{\mathrm{DY}}$ ) is independently measured, and subsequently subtracted from $N_{\gamma \gamma}$, using $Z$ decays to two electrons of which at least one is reconstructed as a photon. Systematic uncertainties in the background decomposition arise from the asymmetry between the photon and the jet transverse energies in photon-jet events, the correlations between isolation and

Table 1: Summary of the number of measured and expected prompt diphoton $\left(N_{\gamma \gamma}\right)$, Drell-Yan $\left(N_{\mathrm{DY}}\right)$, photon-plus-jet $\left(N_{\gamma j}\right)$, and dijet $\left(N_{j j}\right)$ background events with a diphoton invariant mass between 100 and 150 GeV .

|  | $N_{\gamma \gamma}$ | $N_{\mathrm{DY}}$ |
| :---: | :---: | :---: |
| Measured | $219 \pm 25$ (stat.) ${ }_{-9}^{+8}$ (syst.) | $6.7 \pm 0.3$ (stat.) $\pm 1.8$ (syst.) |
| Expected (MC) | $214 \pm 59$ | $7.1 \pm 0.5$ |
|  | $N_{\gamma j}$ | $N_{j j}$ |
| Measured (Reducible) | $59 \pm 12$ (stat.) $\pm 9$ (syst.) | $6 \pm 4$ (stat.) ${ }_{-1}^{+4}$ (syst.) |
| Expected (MC) | $77 \pm 42$ | $2.5 \pm 2.6$ |

identification variables, and the uncertainty in the contribution of diphoton events to the isolation and identification sideband regions. A summary of the main background components, estimated in the 2011 data, is given in Table 1 and illustrated in Figure 1 (a). A reasonable agreement between each measured component and its prediction is observed.

In order to reconstruct the invariant mass of the diphoton system as precisely as possible, two essential ingredients are the photon energy calibration and the reconstruction of the longitudinal position of the primary vertex of the interaction. The calibration of the reconstructed photon energy is based on precise test-beam data as well as on a simulation of the calorimeter and an accurate description of the amount of material upstream of it. This calibration scheme is further completed by an additional correction for energy scale variations as a function of pseudorapidity estimated with electrons from $Z$ decays. As in the 2010 data analysis, for events with more than one reconstructed primary vertex, the vertex associated with tracks having the largest sum of transverse momenta-squared is used to estimate the position of the hard scattering interaction. This method does not use the full ATLAS capabilities to select the primary vertex such as the ability of the calorimeter to determine the photon direction and the reconstruction of converted photons. An improvement in the $\gamma \gamma$ invariant mass resolution of about $10 \%$, in the 2011 data running conditions, compared to the data taken in 2010 [1, 2], could be achieved with a refined primary vertex reconstruction method.

The invariant mass distributions of the events selected in the 2011 data (b) and for the combined 2010 and 2011 data set corresponding to an integrated luminosity of $131 \mathrm{pb}^{-1}$ (c) are shown in Figure 1 along with the absolute background predictions. The expected full width at half maximum (FWHM) of the invariant mass distribution of a narrow resonance decaying into two photons amounts to $\sim 4.5 \mathrm{GeV}[1$, 2]. Given the bin size of 5 GeV in the histograms of Figure 1, if produced at a sufficiently high rate, such a resonance would manifest itself as an excess of events mostly in two bins with respect to their neighboring sidebands. No excess is observed, neither with the analysis criteria described in this note nor with other selections studied.

## Conclusion

The estimate of the background composition in the search for the Higgs boson in the diphoton channel has been updated using a sample of $94 \mathrm{pb}^{-1}$ of data collected in 2011. The main background components are measured and found to be in good agreement with their Standard Model predictions. No excess with respect to the expected backgrounds is observed in the diphoton invariant mass distribution.

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Figure 1: (a) Measured number of events for each background component (points with error bars), compared with the corresponding Monte Carlo predictions (color bands). (b) and (c) Diphoton invariant mass distributions for data and the cumulative predictions of the Drell-Yan (red solid), dijet (blue dotted), photon-jet (blue dashed) and diphoton (blue solid) components of the background for the 2011 data only (b) and the combined 2010 and 2011 data (c). The two yellow bands depict the total uncertainty on the prediction and the uncertainty on the reducible background component only.

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# Search for the Higgs Boson in the Diphoton Channel with the ATLAS Detector using $209 \mathbf{~ p b}^{-1}$ of 7 TeV Data taken in 2011 

The ATLAS collaboration


#### Abstract

This note presents the result of a search for a Higgs boson decaying into a pair of photons in $p p$ collision data collected in 2011 with the ATLAS detector at a centre-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$. In the $209 \mathrm{pb}^{-1}$ of data analysed no statistically significant excess is observed. A $95 \%$ CL exclusion limit on the production cross section of a Higgs boson decaying into two photons relative to the Standard Model cross section is given.


## 1 Introduction

This note presents an update of the search for the Standard Model Higgs boson decaying to two photons. The updated search uses an integrated luminosity of $209 \mathrm{pb}^{-1}$ of $p p$ collision data collected in 2011 by the ATLAS detector [1] at a centre-of-mass energy of 7 TeV at the LHC. Techniques similar to those reported in $[2,3,4]$ are used to estimate the background composition, study the diphoton invariant mass resolution and determine the signal-related systematic uncertainties. Exclusion limits on the $H \rightarrow \gamma \gamma$ rate are derived from the study of the diphoton invariant mass distribution.

## 2 Event Selection and Reconstruction

The data sample collected in 2011 used in this analysis has two distinct LHC bunch patterns, with 75 ns and 50 ns bunch spacings. The vast majority of the data $\left(\sim 194 \mathrm{pb}^{-1}\right)$ was taken in the latter configuration. These conditions were sufficiently similar to not require a special treatment when combined as a single data set. As described in [4] an average number of interactions per bunch crossing of up to $\sim 8$ was reached. A full Monte Carlo simulation, taking into account both the effects of in-time pile-up events, occurring in the same bunch crossing as the hard scattering event, and out-of-time pile-up events, occurring in bunch crossings other than that of the hard scattering process, was used (with both the 50 ns and 75 ns configurations). In the simulation, pile-up events are added to the hard-scattering process according to a Poisson distribution. In order to accurately reproduce the changing beam conditions, the mean value of the Poisson distribution $\left(\mu_{P U}\right)$ is varied, and a reweighting procedure is applied to match the $\mu_{P U}$ distribution of the Monte Carlo to that of the data.

The 2011 data were triggered with the requirement of two photon-candidate clusters selected with loose identification criteria [5] and a transverse energy threshold of 20 GeV on both photons. The trigger efficiency for events passing all selection criteria (described below) is estimated using an independent trigger and is found to be $\sim 99 \pm 1 \%$. Event and object based data quality requirements are applied. Their impact on the signal efficiency are of the order of $\sim 1 \%$.

The kinematic event selection is unchanged with respect to [2, 3, 4]. Diphoton candidates are required to pass tight identification criteria, to be within the inner detector and calorimeter acceptance $(|\eta|<2.37$ excluding $1.37<|\eta|<1.52$ ) and to have transverse momenta larger than 40 GeV and 25 GeV for the leading and sub-leading photons respectively. In this analysis, the diphoton invariant mass range investigated is limited to candidate events with invariant masses between 100 GeV and 150 GeV . The photon identification criteria are essentially the same as those used in [4]. To cope with the higher pile-up environment two basic improvements to the analyses presented in $[2,3,4]$ are made.
(i) The additional pile-up events increase the fluctuations of the photon isolation transverse energy. The isolation requirement is thus relaxed from 3 GeV to 5 GeV . The isolation energy is the energy deposited in a $\Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}=0.4$ cone around the photon in the calorimeters, corrected for the underlying event and pile-up effects on an event-by-event basis, and for out-of-cone showering [6]. This modification resulted in an increase of $\sim 12 \%$ in isolation efficiency per photon and a small reduction in the purity of the diphoton sample from approximately $76 \%$ to $70 \%$.
(ii) Reconstructing the location of the primary vertex (PV) of the hard scattering interaction is crucial for a precise diphoton invariant mass reconstruction. In the moderate pile-up environment of the 2010 data (with an average of $\sim 2$ pile-up events per bunch crossing), the PV location was estimated using the reconstructed PV (from tracks in the inner detector) with the highest sum of the transverse momentum squared of its associated tracks. This choice is not optimal in the current higher pile-up environment. The longitudinal segmentation of the liquid-argon electromagnetic calorimeter and the fine granularity of its first sampling layer can be used to reconstruct the photon
direction, as described in more detail in [7]. The combination of the directions (also referred to as pointing direction) and positions of the two photons is used to estimate the PV location. In addition, when one or both photons are converted, the conversion tracks are also used to locate the PV. As in the case of energy scale and energy resolution, the resolution of the direction measurement is monitored using electrons from $Z$ decays. In the 2011 high pile-up conditions the improvement on the invariant mass resolution using this method amounts to $\sim 5 \%$. The signal diphoton invariant mass distribution for a Higgs boson mass hypothesis of 120 GeV is shown for both PV reconstruction methods in Figure 1. The full width at half maximum of the diphoton mass distribution is 4.1 GeV using the photon directions or conversion tracks.


Figure 1: Distributions of the reconstructed diphoton invariant mass of a simulated 120 GeV Higgs boson signal. Events are produced with a realistic simulation of the photon energy resolution, the effect out-of-time and in-time pile-up events and an inter-bunch spacing of 50 ns . The points and solid fit function correspond to the photon direction or conversion-based PV reconstruction. The triangles and dashed fit function represent the method using the PV with the highest sum of transverse momentum squared. The full width at half maximum of the invariant mass distribution is 4.1 GeV with the method using photon directions and conversion tracks.

After all selection cuts are applied, 926 diphoton candidate events are observed.
The photon identification efficiency is estimated from the Monte Carlo simulation with small shower shape corrections applied to better describe the distributions observed in 2010 data. As in [2, 3, 4], the Monte Carlo isolation efficiency is corrected from data using electrons from $Z$ decays. The smaller inefficiency due to the looser isolation cut reduces the effect of differences between the data and the Monte Carlo simulation.

Applying all selection criteria, for a Higgs boson with a mass between 110 and 140 GeV , the number of expected Standard Model Higgs boson events ranges from 3.6 to 2.5. The main production processes are all accounted for in this estimate, and they include the gluon fusion, the vector boson fusion, and the associated production with a vector boson or a pair of top quarks. Gluon fusion is both dominant and has the largest theoretical uncertainty, despite being computed at an improved next-to-next-to-leading-order level. The cross sections and $\gamma \gamma$ branching fractions used herein were computed in [8]. The uncertainty in the theoretical prediction is estimated to ${ }_{-15}^{+20} \%$ mostly from the renormalisation and factorisation scale variations and the uncertainties in the parton distribution functions [8].

The probability-density function for the signal diphoton mass is modelled by the sum of a Crystal Ball function (for the bulk of the events) and a Gaussian (to model the tails) [3]. Signal events were fully simulated at masses of $110,115,120,130$ and 140 GeV . The parameters of the signal model for Higgs boson mass hypotheses other than those fully simulated are linearly interpolated.

## 3 Background Estimation

The main background components in this analysis are the irreducible prompt diphoton production $(\gamma \gamma)$, the reducible photon-jet process ( $\gamma$-jet), the dijet (jet-jet) processes with one or more fake photons from jets fragmenting mainly into a leading $\pi^{0}$, and Drell-Yan events where both electrons are misidentified as photons. The expected abundance of these background components is indicated in Table 1. The large uncertainties in these predictions mostly arise from the jet fragmentation (into a photon or a leading $\pi^{0}$ ), the parton distribution functions and the variations of renormalisation and factorisation scales in the next-to-leading order predictions [2]. The uncertainty in the Drell-Yan prediction is from the Monte Carlo statistics only. The invariant mass distribution of the 926 candidate events selected in the data is illustrated in Figure 2 (a) along with the Monte-Carlo prediction for each background component.

Altogether the number of expected background events as estimated in [4] and corrected for the difference in the isolation cut is $866 \pm 207$, in agreement with the 926 events observed in the data.

Table 1: Number of expected and measured prompt diphoton ( $N_{\gamma \gamma}$ ), Drell-Yan ( $N_{\mathrm{DY}}$ ), photon-plus-jet $\left(N_{\gamma j}\right)$, and dijet $\left(N_{j j}\right)$ background events with a diphoton invariant mass between 100 GeV and 150 GeV .

|  | $N_{\gamma \gamma}$ | $N_{\text {DY }}$ |
| :---: | :---: | :---: |
| Expected (MC) | $602 \pm 169$ | $18 \pm 2$ (MC stat only) |
| Measured | $643 \pm 45$ (stat.) ${ }_{-71}^{+54}$ (syst.) | $23.8 \pm 0.6$ (stat.) $\pm 3.8$ (syst.) |
| $N_{\gamma j}$ | $N_{j j}$ |  |
| Expected (MC) | $238 \pm 129$ | $8 \pm 8$ |
| Measured (Reducible) | $216 \pm 23$ (stat.) ${ }_{-54}^{+32}$ (syst.) | $43 \pm 6$ (stat.) ${ }_{-18}^{+44}$ (syst.) |

A double side-band method is applied to measure these background components directly from the data as was done in [2, 3, 4]. The treatment of systematic uncertainties is extended to include variations of the base sample selection criteria of the side-band method, resulting in a non-negligible additional systematic uncertainty. The Drell-Yan component, which cannot be distinguished from the irreducible background, is estimated using $Z$ decays to electrons where one electron is misreconstructed as a photon. The results of the background studies are shown in Table 1 and summarised in Figure 2 (b). Good agreement between the data-driven background estimates and the Monte Carlo prediction is observed.

## 4 Systematic Uncertainties

The experimental systematic uncertainty on the event yield has the following main components:
(i) The uncertainty arising from the reconstruction and identification efficiencies amounts to $\pm 11 \%$ per event. It is estimated from data and Monte Carlo differences ( $\pm 5 \%$ per photon as estimated in 2010 data [3]) and the variation of pile-up conditions as a function of $\mu_{P U}$ and the two inter-bunch spacings 50 ns and 75 ns ( $\pm 2 \%$ per photon). The efficiency uncertainties between the two photons in the event are fully correlated.


Figure 2: (a) Diphoton invariant mass distributions for data and the cumulative predictions of the DrellYan (red solid), dijet (blue dotted), photon-jet (blue dashed) and diphoton (blue solid) components of the background. The two yellow bands depict the total uncertainty on the prediction and the uncertainty on the reducible background component only. (b) Measured number of events for each background component (points with error bars), compared with the corresponding Monte Carlo predictions (color bands).
(ii) The uncertainty in the isolation cut efficiency, estimated from the difference in efficiency between data and Monte Carlo found in $Z$ decays to electrons, amounts to $\pm 3 \%$ per event.
(iii) There is a $\pm 1 \%$ uncertainty on the overall event trigger efficiency.
(iv) The preliminary luminosity uncertainty for the 2011 data is $4.5 \%$. It is based on the 2010 luminosity calibration [9] which was transferred to the 2011 data by means of the liquid-argon forward calorimeter and the tile calorimeter current measurements.

The total uncertainty on the overall signal event yield from the event selection, corresponding to the first three sources $(i-i i i)$ listed above, is $\pm 11 \%$. The total experimental uncertainty on the event yield amounts to $\pm 12 \%$.

The uncertainty on the invariant mass resolution has the following main components:
(i) The uncertainty on the constant term of the cluster energy resolution is estimated from $Z$ to electrons decays. It amounts to an $\pm 11 \%$ relative uncertainty on the diphoton invariant mass resolution.
(ii) The uncertainty on the photon energy calibration arising from the extrapolation of the energy scale calibration of electrons, which is then applied to photons, is estimated using a full Monte Carlo simulation with a distorted amount of material upstream of the calorimeter. It amounts to a $\pm 6 \%$ relative uncertainty on the mass resolution.
(iii) The pile-up contributions to the cluster energies are measured in random clusters in events taken at random bunch crossings in the data and compared to the simulation under various pile-up conditions. The impact of the different pile-up contributions on the mass resolution amounts to a $\pm 3 \%$ relative uncertainty.
(iv) The uncertainty on the PV location estimate arising from differences between data and Monte Carlo in the calorimeter photon direction reconstruction is studied in $Z$ to electrons decays and its relative impact on the diphoton invariant mass resolution is $\pm 2 \%$.

The total relative uncertainty on the diphoton invariant mass resolution is $\pm 13 \%$.

## 5 Results

As seen from Figure 2 (a), no significant evidence for an excess in the invariant mass distribution is observed in the data. Using a profile likelihood estimator where the total background is modelled by an exponentially falling distribution determined by two nuisance parameters (the overall background normalisation and its exponential negative slope), and treating the systematic uncertainties on the signal yield and the mass resolution as additional nuisance parameters [3], the data are compared to background and signal-plus-background hypotheses. Within the selected mass range, $100-150 \mathrm{GeV}$, the search is restricted to Higgs boson mass hypotheses between 110 and 140 GeV for which a fit of the signal-plusbackground model to the data is performing well.

The compatibility of the selected events with the background-only hypothesis is quantified by the $1-C L_{b}$ (the probability to observe an excess larger than that observed in the data in the backgroundonly hypothesis) shown in Figure 3 (a) and reported in Table 2. A slight excess is observed at a diphoton invariant mass of $\sim 127 \mathrm{GeV}$. The $1-C L_{b}$ or corresponding $p$-value of the excess is $\sim 2 \%$. The probability for such an excess to occur anywhere in the $110-140 \mathrm{GeV}$ mass range is approximately $30 \%$.

Table 2: The expected Higgs boson signal yields, for fully simulated Higgs boson mass hypotheses with an integrated luminosity of $209 \mathrm{pb}^{-1}$ (the experimental and theoretical uncertainties are given separately). The $1-C L_{b}$ for each of these mass hypotheses and the $95 \%$ CL expected and observed PCL limits on the Higgs production cross section relative to the Standard Model cross section ( $\sigma_{95} / \sigma_{S M}$ ) are also reported. The minimum $1-C L_{b}$ reaches $\sim 2 \%$ for Higgs boson mass hypotheses around $\sim 127 \mathrm{GeV}$.

| Higgs boson mass | $110(\mathrm{GeV})$ | $115(\mathrm{GeV})$ | $120(\mathrm{GeV})$ | $130(\mathrm{GeV})$ | $140(\mathrm{GeV})$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Expected Signal | $3.5 \pm 0.4_{-0.5}^{+0.7}$ | $3.6 \pm 0.4_{-0.5}^{+0.7}$ | $3.6 \pm 0.4_{-0.5}^{+0.7}$ | $3.2 \pm 0.4_{-0.5}^{+0.7}$ | $2.5 \pm 0.3_{-0.4}^{+0.5}$ |
| $1-C L_{b}$ | $55 \%$ | $65 \%$ | $65 \%$ | $10 \%$ | $52 \%$ |
| Expected $\sigma_{95} / \sigma_{S M}$ | 6.9 | 6.5 | 6.4 | 6.0 | 6.9 |
| Observed $\sigma_{95} / \sigma_{S M}$ | 5.7 | 4.2 | 4.6 | 11.7 | 4.9 |

Exclusion limits on the inclusive production cross section of a Standard Model-like Higgs boson relative to the Standard Model cross section are derived. Two interpretations of these limits are given. The first is the purely frequentist $C L_{s+b}$ derived limit for which a power constraint (PCL) is invoked when the observed limit fluctuates more than $-1 \sigma$ from the expected median limit in the backgroundonly hypothesis [10]. This Power Constraint Limit (PCL) interpretation is illustrated in Figure 3 (b). The observed limit does not fluctuate below $-1 \sigma$ from the median expected limit, the power constraint is therefore not invoked. The second, the modified frequentist approach ( $C L_{s}$ method), is illustrated in Figure 3 (c). The results using the PCL method are also summarised in Table 2. The theoretical uncertainty on the predicted Standard Model cross section is not included in the experimental limit but shown as a band around 1 in Figure 3 (b) and (c).

## Conclusion

An update of the $H \rightarrow \gamma \gamma$ analysis with the $209 \mathrm{pb}^{-1}$ of data collected early 2011 is given in this note. Improvements to the analysis were made to cope with the high pile-up environment. The background and signal studies shown in [2,3,4] are repeated here and exclusion limits for Higgs boson mass hypotheses between 110 GeV and 140 GeV are set. In this data sample, expected exclusion limits at $95 \% \mathrm{CL}$ between 6 and 7 times the Standard Model cross section are achieved. The observed excluded cross section of a Standard Model-like Higgs boson decaying into a pair of photons ranges between 4.2 and 15.8 times the

Standard Model cross section. The fluctuations of this observed limit are compatible with the expected statistical fluctuations of the background.

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Figure 3: (a) $1-C L_{b}$ as a function of the Higgs boson mass hypothesis. Exclusion limits using the PCL (b) and $C L_{s}$ methods (c) on the production cross section relative to the Standard Model cross section as a function of Higgs mass hypothesis.

ATLAS NOTE
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# Search for technihadrons in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS detector 

The ATLAS Collaboration


#### Abstract

A search for the technivector mesons $\rho_{T}$ and $\omega_{T}$ produced in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ and decaying to dielectron and dimuon final states is presented. The analysis is based on $1.08 \mathrm{fb}^{-1}\left(1.21 \mathrm{fb}^{-1}\right)$ of data for the $e e(\mu \mu)$ channel collected with the ATLAS detector at the CERN LHC. Since the $\rho_{T}$ and $\omega_{T}$ are narrow, spin 1 resonances, the search uses the limit results of the ATLAS $Z^{\prime}$ search. No evidence for a technihadron signal is observed. Within the context of the low-scale technicolor model, masses of the $\rho_{T}$ and $\omega_{T}$ from 130-480 GeV are excluded at $95 \% \mathrm{CL}$ for $\pi_{T}$ masses from $50-480 \mathrm{GeV}$.


Technicolor (TC) models use new strong dynamics to provide an alternative mechanism for breaking electroweak symmetry. In contrast to the Standard Model Higgs mechanism, TC avoids the introduction of fundamental scalar particles. Technicolor models predict new technihadron states that could be copiously produced at the LHC. The lowest mass states are the scalar technipion $\pi_{T}^{ \pm, 0}$ and the vector technirho $\rho_{T}^{ \pm, 0}$ and techniomega $\omega_{T}^{0}$. These technivector mesons can decay into a Standard Model (SM) gauge boson plus technipion $\left(\gamma \pi_{T}, W \pi_{T}\right.$ or $Z \pi_{T}$ ), pairs of SM gauge bosons ( $W Z, \gamma W$, etc.) and fermion-antifermion pairs.

A search for the $\rho_{T}$ and $\omega_{T}$ in the dilepton final state has been conducted previously by CDF and placed a lower bound on the $\rho_{T}$ and $\omega_{T}$ masses of 280 GeV [1]. A recent search by CDF [2] for technihadrons in the $W \pi_{T}$ final state excludes a region of the $m\left(\rho_{T}\right)-m\left(\pi_{T}\right)$ plane where $m\left(\rho_{T}\right)$ ranges from 180250 GeV and $m\left(\pi_{T}\right)$ from $95-145 \mathrm{GeV}$. Another recent search in the $W Z$ final state by $\mathrm{D} \emptyset[3]$ rules out the interval of $\rho_{T}$ mass from $208-408 \mathrm{GeV}$ when the $W Z$ mode is dominant, i.e. when $m\left(\rho_{T}\right)<m\left(\pi_{T}\right)+m(W)$. A similar search in the $W Z$ final state by CMS [4] excluded $\rho_{T}$ masses below 436 GeV .

Additional motivation for this search stems from the observation by CDF of an excess in the dijet mass spectrum in $W j j$ events [5]. It has led to speculation that the excess may be due to a $290 \mathrm{GeV} \rho_{T}$ that decays into a $W$ and a $160 \mathrm{GeV} \pi_{T}$ [6].

In this note a search for the technicolor vector mesons $\rho_{T}$ and $\omega_{T}$ with their subsequent decay to $\ell^{+} \ell^{-}$, where $\ell=e$ or $\mu$, is presented. The search is performed in the context of the low-scale technicolor model (LSTC) [7, 8]. In the LSTC model, it is assumed that techni-isospin is a good symmetry and therefore the isotriplet $\rho_{T}$ and isosinglet $\omega_{T}$ will be nearly degenerate in mass. For what follows, it is assumed that $m\left(\rho_{T}\right)=m\left(\omega_{T}\right)$ and therefore the signal in the dilepton mass spectrum is the sum of the $\rho_{T}$ and $\omega_{T}$ contributions. The $\omega_{T}$ branching ratio to dileptons is approximately an order of magnitude larger than for the $\rho_{T}$ so the dilepton signal is mostly due to the $\omega_{T}$. The natural width of the $\rho_{T}$ and $\omega_{T}$ resonances is very narrow, less that 1 GeV , so that the observed line shape is due to detector resolution alone. Other important LSTC parameters are the number of technicolors $N_{T C}=4$, the charges of the up (U) and down (D) type technifermions $Q_{U}=Q_{D}+1=1$, the mixing angle $\sin \chi=1 / 3$, and the vector and axial mass parameters $M_{V}=M_{A}=m\left(\rho_{T}\right)$.

Since the $\rho_{T}$ and $\omega_{T}$ are narrow, spin 1 resonances, the search methodology will be identical to that developed for the ATLAS search for the $Z^{\prime} \rightarrow \ell^{+} \ell^{-}$where $\ell=e$ or $\mu$ [9]. The same data samples, object identification and event selection criteria, backgrounds, and systematic uncertainty determination as presented in Ref. [9] were used here.

The $\rho_{T}$ and $\omega_{T}$ signal cross sections were calculated with Pythia 6.4 [10] using MRST2007 LO* parton density functions (PDF) [11]. A dilepton-mass-dependent K-factor was applied to account for higher order QCD effects [9].

To demonstrate that the $Z^{\prime} 95 \%$ CL cross section limit results may be used directly for the TC search, it is sufficient to show that the kinematics and acceptance are the same for the $Z^{\prime}$ and TC signals. Figure 1 plots the acceptance times efficiency $(A \epsilon)$ as a function of dielectron mass for the $\rho_{T} / \omega_{T}$ and $Z^{\prime}$. Figure 2 plots $A \epsilon$ for the dimuon channel. The results agree within the statistical uncertainty and therefore the $Z^{\prime}$ limits from Ref. [9] may be used unaltered for setting limits on TC.

Figure 3 shows the dielectron mass distribution from $1.08 \mathrm{fb}^{-1}$ of 2011 data along with the expected SM backgrounds and representative TC signals. Figure 4 shows the analogous plot for the dimuon channel obtained from $1.21 \mathrm{fb}^{-1}$ of 2011 data. The agreement between data and SM backgrounds is excellent and quantified in Ref. [9].

In the absence of a TC signal, limits on the cross section times dilepton branching ratio are set as a function of resonance mass. Within the context of the LSTC model, the limit on $\sigma B\left(\ell^{+} \ell^{-}\right)$is converted into a lower limit on the mass of the $\rho_{T} / \omega_{T}$. Figure 5 plots the $95 \% \mathrm{CL}$ observed and expected exclusion regions in the $m\left(\pi_{T}\right)-m\left(\rho_{T} / \omega_{T}\right)$ plane. The mass limit depends on the $\rho_{T} / \omega_{T}-\pi_{T}$ mass splitting since that determines if decay modes such as $W \pi_{T}$ or multi- $\pi_{T}$ are kinematically allowed. Masses of the $\rho_{T}$


Figure 1: Signal acceptance times efficiency as a function of dielectron mass for the $\rho_{T} / \omega_{T}$ and for the $Z^{\prime}$.


Figure 2: Signal acceptance times efficiency as a function of dimuon mass for the $\rho_{T} / \omega_{T}$ and for the $Z^{\prime}$.


Figure 3: The dielectron mass distribution after the final event selection showing the data in points and the SM backgrounds from the $Z / \gamma^{*}$, diboson, $t \bar{t}, W+$ jets, and QCD multijet processes in stacked filled histograms. Also shown in open histograms is the expected LSTC signal for several $\rho_{T} / \omega_{T}$ masses.


Figure 4: The dimuon mass distribution after the final event selection showing the data in points and the SM backgrounds from the $Z / \gamma^{*}$, diboson, $t \bar{t}$, $W+$ jets, and QCD multijet processes in stacked filled histograms. Also shown in open histograms is the expected LSTC signal for several $\rho_{T} / \omega_{T}$ masses.


Figure 5: The $95 \%$ CL excluded region as a function of the assumed $\pi_{T}$ and $\rho_{T} / \omega_{T}$ masses is shown in red. The dotted line corresponds to $m\left(\rho_{T} / \omega_{T}\right)-m\left(\pi_{T}\right)=100 \mathrm{GeV}$. The dashed line shows the expected limit with the green dashed lines showing the $\pm 1 \sigma$ bands. The hashed region where $m\left(\pi_{T}\right)>m\left(\rho_{T} / \omega_{T}\right)$ is excluded by theory. Also shown are recent results from CDF [2] and DØ [3].


Figure 6: The expected and observed $95 \%$ CL limits on $\sigma B$ as a function of mass of $\rho_{T} / \omega_{T}$ or $Z^{\prime}$ for the combination of the dielectron and dimuon channels. Also shown are the theory predictions for the LSTC model, assuming $m\left(\rho_{T} / \omega_{T}\right)-m\left(\pi_{T}\right)=100 \mathrm{GeV}$, and for the $Z^{\prime}$ models studied in Ref. [9]. The thickness of the theory curves illustrate the theoretical uncertainties, which for the $Z^{\prime}$ curves are described in Ref. [9] and for the LSTC curve are the PDF and K-factor uncertainties.
and $\omega_{T}$ from $130-480 \mathrm{GeV}$ are excluded at $95 \% \mathrm{CL}$ for $\pi_{T}$ masses from $50-480 \mathrm{GeV}$. Figure 6 plots the $95 \%$ CL observed and expected limits on $\sigma B\left(\ell^{+} \ell^{-}\right)$as a function of mass of the $\rho_{T} / \omega_{T}$ or $Z^{\prime}$ resonance. For an assumed $\rho_{T} / \omega_{T}-\pi_{T}$ mass splitting of 100 GeV , masses of the $\rho_{T}$ and $\omega_{T}$ below 470 GeV are excluded at $95 \% \mathrm{CL}$.

To conclude, a search for the technivector mesons $\rho_{T}$ and $\omega_{T}$ in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ has been presented. The search methodology is identical to that used for the ATLAS $Z^{\prime} \rightarrow e^{+} e^{-}$and $Z^{\prime} \rightarrow$ $\mu^{+} \mu^{-}$searches [9]. No evidence for a TC signal is observed in $1.08 \mathrm{fb}^{-1}\left(1.21 \mathrm{fb}^{-1}\right)$ of data for the $e e$ $(\mu \mu)$ channel. The results of Ref. [9] are used to exclude at $95 \%$ CL masses of the $\rho_{T}$ and $\omega_{T}$ from $130-480 \mathrm{GeV}$ for $\pi_{T}$ masses from $50-480 \mathrm{GeV}$.

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## Appendices

## A Extra Public Plots



Figure 7: Comparison of the generator level $p_{T}$ distributions for the $\rho_{T} / \omega_{T}$ (red) and the $Z^{\prime}$ (blue) for the leading $p_{\mathrm{T}}$ lepton (top) and subleading lepton (bottom). In the ratio the $\rho_{T} / \omega_{T}$ distributions are divided by those of the $Z^{\prime}$. The $\rho_{T} / \omega_{T}$ and the $Z^{\prime}$ resonance masses are all 250 GeV .


Figure 8: Comparison of the generator level $\eta$ (top) and $\phi$ (bottom) distributions for the $\rho_{T} / \omega_{T}$ (red) and the $Z^{\prime}$ (blue). In the ratio the $\rho_{T} / \omega_{T}$ distributions are divided by those the $Z^{\prime}$. The $\rho_{T} / \omega_{T}$ and the $Z^{\prime}$ resonance masses are all 250 GeV .


Figure 9: The expected and observed $95 \%$ CL limits on $\sigma B$ as a function of mass of $\rho_{T} / \omega_{T}$ for the dielectron channel. Also shown is the LSTC cross section assuming $m\left(\rho_{T} / \omega_{T}\right)-m\left(\pi_{T}\right)=100 \mathrm{GeV}$. The thickness of the LSTC theory curve illustrates the effect of the PDF and K-factor uncertainties.

Table 1: Excluded ranges of $\rho_{T} / \omega_{T}$ mass at $95 \% \mathrm{CL}$ from the dielectron, dimuon and dilepton channels, assuming $m\left(\rho_{T} / \omega_{T}\right)-m\left(\pi_{T}\right)=100 \mathrm{GeV}$.

| Channel | Observed mass exclusion [GeV] | Expected mass exclusion [GeV] |
| :---: | :---: | :---: |
| $\rho_{T} / \omega_{T} \rightarrow e^{+} e^{-}$ | $m<323$ and $386<m<445$ | $m<345$ |
| $\rho_{T} / \omega_{T} \rightarrow \mu^{+} \mu^{-}$ | $m<280$ and $304<m<376$ | $m<330$ |
| $\rho_{T} / \omega_{T} \rightarrow \ell^{+} \ell^{-}$ | $m<470$ | $m<442$ |



Figure 10: The expected and observed $95 \%$ CL limits on $\sigma B$ as a function of mass of $\rho_{T} / \omega_{T}$ for the dimuon channel. Also shown is the LSTC cross section assuming $m\left(\rho_{T} / \omega_{T}\right)-m\left(\pi_{T}\right)=100 \mathrm{GeV}$. The thickness of the LSTC theory curve illustrates the effect of the PDF and K-factor uncertainties.


Figure 11: The $95 \%$ CL excluded region as a function of the assumed $\pi_{T}$ and $\rho_{T} / \omega_{T}$ masses is shown in red. The dashed line shows the expected limit with the green dashed lines showing the $\pm 1 \sigma$ bands. The hashed region where $m\left(\pi_{T}\right)>m\left(\rho_{T} / \omega_{T}\right)$ is excluded by theory.


Figure 12: The ratio of the $95 \%$ CL exclusion cross-section $\sigma_{\text {limit }}$ and the theoretical cross-section $\sigma_{T h}$ is plotted versus mass of the corresponding resonance in $Z^{\prime}$ models and the LSTC model. The $\sigma_{T h}$ for the LSTC model assumes $m\left(\rho_{T} / \omega_{T}\right)-m\left(\pi_{T}\right)=100 \mathrm{GeV}$.


Figure 13: The ratio of the cross-section $\sigma_{\text {model } X}$ of model $X$ (where $X=L S T C, Z_{\chi}^{\prime}, Z_{\psi}^{\prime}$ ) and the $Z_{S S M}^{\prime}$ cross-section $\sigma_{Z_{S S M}^{\prime}}$ is plotted versus the $Z_{S S M}^{\prime}$ mass. Overlaid is the ratio of the $95 \%$ CL exclusion cross-section $\sigma_{\text {limit }}$ and the $Z_{S S M}^{\prime}$ cross-section $\sigma_{Z_{S S M}^{\prime}}$. The $\sigma_{\text {model } X}$ for the LSTC model assumes $m\left(\rho_{T} / \omega_{T}\right)-m\left(\pi_{T}\right)=100 \mathrm{GeV}$.

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# Search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ with the ATLAS detector 

The ATLAS collaboration


#### Abstract

The search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow$ $\ell^{+} \ell^{-} \ell^{+} \ell^{-}$, where $\ell=e, \mu$, is presented. Proton-proton collision data at $\sqrt{s}=7 \mathrm{TeV}$ recorded with the ATLAS detector and corresponding to an average integrated luminosity of $1.1 \mathrm{fb}^{-1}$ are compared to the Standard Model expectations. Upper limits on the production cross section of a Standard Model Higgs boson with a mass between 110 and 600 GeV are derived. The observed (expected) $95 \%$ confidence level upper limit on the production cross section for a Higgs boson with a mass of 200 GeV , near the most sensitive point of this search, is 2.0 (1.7) times the Standard Model prediction.


## 1 Introduction

The search for the Standard Model (SM) Higgs boson [1-3] is a major goal of the Large Hadron Collider (LHC) programme. Direct searches at the CERN LEP $e^{+} e^{-}$collider have led to a lower limit on the Higgs boson mass, $m_{H}$, of 114.4 GeV at $95 \%$ confidence level (CL) [4]. The searches at the Fermilab Tevatron $p \bar{p}$ collider have excluded at $95 \%$ CL the region $158 \mathrm{GeV}<m_{H}<173 \mathrm{GeV}$ [5]. Results from the 2010 LHC run extended the search in the region $200 \mathrm{GeV}<m_{H}<600 \mathrm{GeV}$ by excluding a SM Higgs boson with cross section larger than 5-20 times the SM prediction [6, 7].

This note presents the search by the ATLAS experiment for the SM Higgs boson in the channel $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{\prime}+\ell^{\prime-}$, where $\ell, \ell^{\prime}=e, \mu$, in the mass range from 110 to 600 GeV . Three distinct final states, $\mu \mu \mu \mu(4 \mu), e e \mu \mu(2 e 2 \mu)$, and eeeee $(4 e)$, are selected. The largest background to this search comes from the $Z Z^{(*)}$ production. For $m_{H}<180 \mathrm{GeV}$, contributions from $Z+$ jets and $t \bar{t}$ processes, where the additional leptons arise either from semi-leptonic decays of heavy flavour or light jets misidentified as leptons, are important. The proton-proton collision data were recorded with the ATLAS detector at the LHC at $\sqrt{s}=7 \mathrm{TeV}$ and correspond to an average integrated luminosity of $1.1 \mathrm{fb}^{-1}$ [8]. The previously published ATLAS results in this channel [6] are improved by using about 27 times more integrated luminosity.

## 2 The ATLAS Detector

The ATLAS detector [9] is a multipurpose particle physics apparatus with forward-backward symmetric cylindrical geometry ${ }^{1}$. The inner tracking detector (ID) consists of a silicon pixel detector, a silicon microstrip detector, and a transition radiation tracker. The ID is surrounded by a thin superconducting solenoid providing a 2 T magnetic field. A high-granularity lead-liquid-Argon (LAr) sampling calorimeter measures the energy and the position of electromagnetic showers. An iron-scintillator tile calorimeter provides hadronic coverage in the central rapidity range. The end-cap and forward rapidity regions are instrumented with LAr calorimetry for both electromagnetic and hadronic measurements. The muon spectrometer (MS) surrounds the calorimeters and consists of three large superconducting toroids, each with eight coils, a system of precision tracking chambers, and detectors for triggering. A three-level trigger system selects events to be recorded for offline analysis.

## 3 Data and Monte Carlo Samples

The accumulated data are subjected to quality requirements ensuring that the relevant detector components are operational. The average integrated luminosity of $1.1 \mathrm{fb}^{-1}$ corresponds to $1.21 \mathrm{fb}^{-1}, 1.07 \mathrm{fb}^{-1}$, and $1.07 \mathrm{fb}^{-1}$ for the $4 \mu, 2 e 2 \mu$, and $4 e$ final states respectively.

The $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ signal is modelled in the range 110 to 600 GeV using the powheg Monte Carlo (MC) event generator [10, 11], which calculates separately the gluon and vector-boson fusion production mechanisms of the Higgs boson with matrix elements up to next-to-leading order (NLO). The Higgs boson $p_{\mathrm{T}}$-spectrum is reweighted to the calculation of ref. [12], correseponding to QCD corrections up to next-to-leading order and QCD soft-gluon resummations up next-to-next-to-leading log. POWHEG is interfaced to PYTHIA [13] for showering and hadronization, which in turn is interfaced to PHOTOS [14] for QED radiative corrections in the final-state and to TAUOLA [15,16] for the simulation of $\tau$ decays. The

[^62]Higgs boson $p_{\mathrm{T}}$ spectrum is reweighted to the calculation of Ref. [12], corresponding to QCD corrections up to next-to-leading order and QCD soft-gluon resummations up next-to-next-to-leading log.

The cross sections for Higgs boson production, the corresponding branching fractions, as well as their uncertainties, are compiled in Ref. [17]. They correspond to next-to-next-to-leading order (NNLO) in QCD for the gluon fusion [18-23] and vector boson fusion [24]. In addition, QCD soft-gluon resummations up to next-to-next-to-leading $\log$ (NNLL) are available for the gluon fusion process [25], while the NLO electroweak (EW) corrections are applied to both the gluon fusion [26,27] and vector boson fusion [28,29]. The Higgs boson decay branching ratio to the four-lepton final state is predicted by PROPHECY4F [30,31], including the complete NLO QCD+EW corrections, including all interference effects and leading two-loop heavy Higgs boson corrections to the four-fermion width. Table 1 gives the production cross-sections for the $H \rightarrow 4 \ell(\ell=e, \mu)$ for typical Higgs boson masses.

Table 1: Higgs boson production cross-sections for both gluon and vector-boson fusion processes in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$. The cross-sections include the branching ratio of $H \rightarrow 4 \ell, \ell=e, \mu$.

| $m_{H}(\mathrm{GeV})$ | 130 | 150 | 200 | 240 | 300 | 400 | 500 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\sigma \cdot \mathrm{BR}(H \rightarrow 4 \ell)(\mathrm{fb})$ | 2.87 | 4.38 | 6.77 | 5.35 | 3.75 | 2.66 | 1.11 |

The $Z Z^{(*)}$ background is generated using PYTHIA, taking into account $Z-\gamma$ interference. For the inclusive total cross section and the shape of the $m_{Z Z^{(*)}}$ spectrum the MCFM [32,33] prediction is used, including both quark-antiquark annihilation at QCD NLO and gluon fusion. Inclusive $Z$ boson and $Z b \bar{b}$ processes are modelled using ALPGEN [34], removing overlaps between the two samples. More specifically, $b \bar{b}$ pairs with separation $\Delta R=\sqrt{\Delta \phi^{2}+\Delta \eta^{2}} \geq 0.4$ between the jets are taken from the matrix-element calculation, while for $\Delta R<0.4$ the parton-shower jets are used. The total inclusive cross section for $Z$ boson production is normalized to the QCD NNLO prediction by FEWZ [35, 36], while $Z b \bar{b}$ is normalized to the MCFM prediction [32,33]. Finally, the $t \bar{t}$ background is modelled using MC @ NLO [37] and is normalized to the approximate NNLO cross section calculated using HATHOR [38]. Both ALPGEN and MC@NLO are interfaced to HERWIG [39] for parton shower hadronization and to JIMMY [40] for the underlying event simulations.

All generated events undergo a full detector simulation performed using GEANT4 [41, 42].
As a result of the intensity increase of LHC an average number of five interactions per bunch crossing has been measured in data. In order to adequately take into account the impact of pileup on lepton reconstruction efficiency and isolation, these effects have been included in all ATLAS simulations.

## 4 Physics Object Identification and Event Selection

The data were collected using single-lepton triggers with thresholds on transverse energy, $\mathrm{E}_{T}$, of 20 GeV for electrons and on transverse momentum, $p_{\mathrm{T}}$, of 18 GeV for muons. Both triggers are more than $99.5 \%$ efficient for events passing the selection described below.

Electron candidates consist of clusters of energy deposited in the electromagnetic calorimeter associated to inner detector tracks. The electrons must satisfy the ATLAS "medium" electron criteria that require the shower profiles to be consistent with those expected from an electromagnetic shower shape and a well reconstructed ID charged track pointing to the corresponding clusters [43].

Muon candidates are reconstructed by matching inner detector tracks with either full or partial tracks in the muon spectrometer [44-46]. For the former case, the two independent momentum measurements are combined, while for the latter case the muon spectrometer provides only the muon identification
information. To reject cosmic rays, tracks are required to be consistent with having originated from the primary vertex, defined as the reconstructed vertex with the highest $\sum p_{\mathrm{T}}^{2}$ of associated tracks.

Leptons from Higgs boson decays are expected to be isolated and to originate from a common vertex. Track and calorimeter isolation as well as transverse impact parameter significance requirements are therefore applied to further reduce the $Z+$ jets and $t \bar{t}$ contributions. The sum of $p_{\mathrm{T}}$ of tracks within $\Delta R<0.20$ from the lepton divided by the lepton $p_{\mathrm{T}}$ is required to be less than 0.15 , while the sum $E_{\mathrm{T}}$ of the calorimeter cells within $\Delta R<0.20$ around the lepton divided by the lepton $p_{\mathrm{T}}$ is required to be less than 0.30 . In the case of electrons, the calorimeter cells corresponding to the electromagnetic shower are subtracted from the cone. The cut on the impact parameter significance is tuned to guarantee more than $95 \%$ efficiency for an isolated lepton. The selection efficiency of the isolation and impact parameter requirements has been studied using data both for isolated leptons, with $Z \rightarrow \ell \ell$ events, and non-isolated leptons from semi-leptonic heavy flavour decays, with heavy-flavour enriched dijet sample, and found to be well described by the simulation.

Higgs boson candidates are formed by selecting two same-flavour, opposite-sign isolated lepton pairs in an event. Each lepton must satisfy $p_{\mathrm{T}}>7 \mathrm{GeV}$ and be measured in the pseudorapidity range $|\eta|<$ 2.47 for electrons and $|\eta|<2.5$ for muons. For the transition region between the barrel and the end-cap calorimeters $1.37<\eta<1.52$, the electron $p_{\mathrm{T}}$ threshold is increased to 15 GeV . At least two leptons must have $p_{\mathrm{T}}>20 \mathrm{GeV}$. The leptons are required to be well separated from each other, $\Delta R>0.1$. The invariant mass of the lepton pair closest to the nominal $Z$ boson mass $\left(m_{Z}\right)$ is denoted by $m_{12}$. It is required that $\left|m_{Z}-m_{12}\right|<15 \mathrm{GeV}$. The invariant mass of the remaining lepton pair, $m_{34}$, is required to be greater than a threshold depending on the reconstructed four lepton mass, $m_{4 \ell}$, as summarized in Table 2. The final discriminating variable is $m_{4 \ell}$, where the Higgs boson production would appear as a clustering of events on top of the background.

Table 2: Summary of thresholds applied to $m_{34}$ for reference values of $m_{4 \ell}$. For other $m_{4 \ell}$ values, the selection requirement is obtained with linear interpolation.

| $m_{4 \ell}(\mathrm{GeV})$ | $\leq 120$ | 130 | 140 | 150 | 160 | 165 | 180 | 190 | $\geq 200$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| threshold $(\mathrm{GeV})$ | 15 | 20 | 25 | 30 | 30 | 35 | 40 | 50 | 60 |

## 5 Background Estimation

The dominant $Z Z^{(*)}$ background is estimated using MC simulation. Generated events are required to pass the complete analysis selection and the final rate is normalized to the integrated luminosity.

The $t \bar{t}$ background is also estimated using MC simulation. Comparing data to MC predictions in a control sample of opposite sign electron-muon pairs consistent with the $Z$ boson mass and with one or two additional leptons, verifies that the $t \bar{t}$ background is small with respect to the dominant $Z Z^{(*)}$ process and under control.

The $Z+j$ jets background is normalized on a data control sample. The control sample is formed by selecting events with a pair of same-flavour, opposite-sign isolated leptons consistent with the $Z$ boson mass, $\left|m_{Z}-m_{12}\right|<15 \mathrm{GeV}$, and a second same-flavour, opposite-sign lepton pair where only kinematic, but no isolation or impact parameter, requirements are applied. At this stage, the dominant background source depends on the flavour of the second lepton pair: $Z b \bar{b}$ production dominates the final states with a second muon-pair and $Z+$ light jets the final states with a second electron-pair. In Fig. 1 distributions of the number of additionnal muons in events with a reconstructed $Z \rightarrow \ell \ell$ decay and of their transverse momentum are compared with MC expectations. The small contributions from $t \bar{t}, Z Z^{(*)}$, and muons


Figure 1: (a) Multiplicity with $p_{T}>7 \mathrm{GeV}$ and (b) $p_{T}$ distribution of additional muons in events with a reconstructed $Z \rightarrow \ell \ell$ decay, $\left|m_{Z}-m_{12}\right|<15 \mathrm{GeV}$, before and after the subtraction of muons originating from light quarks and $Z Z, W Z$ and $t \bar{t}$ decays. The Monte Carlo expectation for the heavy flavour component, $Q$, is also presented. The quoted uncertainties include both statistical and systematic effects.
from in-flight $\pi$ and $K$ decays are subtracted. The yield of the background, which is found to be in good agreement with expectation, is extrapolated to the signal region by means of the MC simulation.

## 6 Systematic Uncertainties

Uncertainties on lepton reconstruction and identification efficiency, momentum resolution and momentum scale are constrained using the accumulated samples of $W / Z$ bosons and $J / \psi$ decays. The muon efficiency uncertainty results in an acceptance uncertainty on the signal and the irreducible background which is uniform over the mass range of interest and amounts to $1.7 \%(1.2 \%)$ for the $4 \mu(2 e 2 \mu)$ channel. The electron efficiency for the $4 e(2 e 2 \mu)$ channel results in an acceptance uncertainty of $3 \%(2 \%)$ at $m_{4 \ell}=600 \mathrm{GeV}$ and reaches $15 \%(6 \%)$ at $m_{4 \ell}=110 \mathrm{GeV}$ for the $4 e(2 e 2 \mu)$ channel.

A conservative theoretical uncertainty of $15 \%$ is assigned to the $Z Z^{(*)}$ background contribution [47]. The $Z+$ jets and $Z b \bar{b}$ contributions to the four lepton final state are evaluated on data. A systematic uncertainty between $20 \%$ and $40 \%$ is assigned on the normalization to account for the statistical uncertainty in the control sample and the extrapolation to the signal region. The uncertainty on the $t \bar{t}$ cross section is found to be $10 \%$ by adding linearly the contributions from variations of the scale and of the parton distribution functions.

The theoretical uncertainties on the Higgs boson production cross section are 15-20\% for the gluon fusion process and $3-9 \%$ for the vector-boson fusion process [17], depending on the Higgs boson mass ${ }^{2}$. These errors are composed of uncertainties in QCD scale and parton distribution functions [49-52]. An additional $2 \%$ uncertainty is added to the signal selection efficiency due to the modelling of the signal kinematics. This is evaluated by comparing signal samples generated with PYTHIA instead of POWHEG.

[^63]Table 3: The expected number of signal and background events, with their systematic uncertainty, separated into "Low mass" ( $m_{4 \ell}<180 \mathrm{GeV}$ ) and "High mass" ( $m_{4 \ell} \geq 180 \mathrm{GeV}$ ) regions. The observed number of events is also presented.

|  | $\mu \mu \mu \mu$ |  | ee $\mu \mu$ |  | eeee |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Low mass | High mass | Low mass | High mass | Low mass | High mass |
| $Z Z^{(*)}$ | $0.84 \pm 0.13$ | $4.5 \pm 0.7$ | $0.80 \pm 0.12$ | $5.6 \pm 0.8$ | $0.33 \pm 0.07$ | $2.1 \pm 0.3$ |
| $Z, Z b \bar{b}$, and $t \bar{t}$ | $0.03 \pm 0.01$ | $0.01 \pm 0.01$ | $0.15 \pm 0.06$ | $0.08 \pm 0.03$ | $0.12 \pm 0.05$ | $0.07 \pm 0.03$ |
| Total Background | $0.87 \pm 0.13$ | $4.5 \pm 0.7$ | $0.95 \pm 0.13$ | $5.7 \pm 0.8$ | $0.45 \pm 0.09$ | $2.2 \pm 0.3$ |
| Data | 1 | 9 | 1 | 5 | 0 | 2 |
| $m_{H}=130 \mathrm{GeV}$ | $0.21 \pm 0.03$ |  | $0.21 \pm 0.03$ |  | $0.07 \pm 0.01$ |  |
| $m_{H}=150 \mathrm{GeV}$ | $0.50 \pm 0.08$ |  | $0.50 \pm 0.08$ |  | $0.18 \pm 0.03$ |  |
| $m_{H}=200 \mathrm{GeV}$ |  | $1.18 \pm 0.17$ |  | $1.40 \pm 0.20$ |  | $0.50 \pm 0.07$ |
| $m_{H}=240 \mathrm{GeV}$ |  | $0.90 \pm 0.13$ |  | $1.16 \pm 0.17$ | $0.46 \pm 0.07$ |  |
| $m_{H}=300 \mathrm{GeV}$ |  | $0.60 \pm 0.09$ |  | $0.85 \pm 0.12$ | $0.33 \pm 0.05$ |  |
| $m_{H}=400 \mathrm{GeV}$ |  | $0.44 \pm 0.07$ |  | $0.64 \pm 0.10$ | $0.27 \pm 0.04$ |  |
| $m_{H}=600 \mathrm{GeV}$ |  | $0.08 \pm 0.01$ |  | $0.12 \pm 0.02$ |  | $0.05 \pm 0.01$ |

The overall uncertainty for the total integrated luminosity is $3.7 \%$ [8].

## 7 Results

Table 3 shows the number of events observed in each final state, separately for $m_{4 \ell}<180 \mathrm{GeV}$ and $m_{4 \ell} \geq 180 \mathrm{GeV}$, compared with the expectations for background. The expected signal yields for various $m_{H}$ values are also presented. In total 18 candidate events are selected by the analysis: ten $4 \mu$, six $2 e 2 \mu$, and two $4 e$ events. In the same mass range 14.6 events are expected from the described background processes. The mass spectra for $m_{12}, m_{34}$, and $m_{4 \ell}$ are shown in Fig. 2, while the kinematic distributions of the leptons are presented in Fig. 3 and Fig. 4. The selected events have been examined visually and no reconstruction issues were identified. Typical event displays are presented in Figs. 5, 6, 7. In Fig. 8, the $m_{4 \ell}$ distribution is shown along with the expected background and the expected signal for several $m_{H}$ hypotheses.

Upper limits are set on the Higgs boson cross section at $95 \% \mathrm{CL}$, using the $C L_{s}$ modified frequentist formalism [53] with the profile likelihood test statistic [54]. Figure 9 shows the expected and observed exclusions as a function of $m_{H}$ and Table 4 summarizes the numerical values for selected $m_{H}$ points. The consistency with the background-only hypothesis is quantified using the $p$-value, the probability that a background-only experiment will fluctuate more than a given observation. The most significant deviation from the background-only hypothesis is observed at $m_{H}=246 \mathrm{GeV}$ with a $p$-value of $3 \%$. This calculation does not account for the look-elsewhere effect.

## 8 Summary

The search for the decay $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ in the data accumulated by the ATLAS detector corresponding to $1.1 \mathrm{fb}^{-1}$ has been presented. No significant excess of candidates is observed in the mass range between 110 and 600 GeV with respect to the expected SM background. The observed (expected) 95\% CL upper


Figure 2: Invariant mass distributions (a) $m_{12}$, (b) $m_{34}$, and (c) $m_{4 \ell}$ for the selected candidates. All plots show comparisons with background expectation from the dominant $Z Z^{*}$ and the sum of $t \bar{t}, Z b \bar{b}$ and $Z+j e t s$ processes. Error bars represent $68.3 \%$ central confidence intervals.


Figure 3: $p_{T}$ distribution (a) and $\eta$ distribution (b) for the leptons of the 18 candidates surviving the selection criteria. The corresponding shapes for the expected background contributions are also shown.
limit on the Higgs boson production cross section, in units of the SM rate, is 2.0 (1.7) at $m_{H}=200 \mathrm{GeV}$, which is the most sensitive point of this search.


Figure 4: Scatter plot of $m_{12}$ and $m_{34}$ for the 18 candidates surviving the selection criteria. The corresponding shape for the total expected background contribution is also shown.


Figure 5: Event display of a $4 e$ candidate event with $m_{4 l}=270.1 \mathrm{GeV}$. The masses of the lepton pairs are 85.0 and 111.3 GeV respectively.


Figure 6: Event display of a $4 \mu$ candidate event with $m_{4 l}=143.5 \mathrm{GeV}$. The masses of the lepton pairs are 90.6 and 47.4 GeV respectively.


Figure 7: Event display of a $2 e 2 \mu$ candidate event with $m_{4 l}=209.7 \mathrm{GeV}$. The masses of the lepton pairs are 85.9 and 85.5 GeV respectively.


Figure 8: $m_{4 \ell}$ distribution of the selected candidates, compared to the background expectation. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown. The resolution of the reconstructed Higgs mass is dominated by experimental performances at low $m_{H}$ values and by the natural Higgs boson width at high $m_{H}$.

Table 4: Observed and median expected 95\% CL upper limit on the SM Higgs boson production cross section, in multiples of the SM rate, as a function of the Higgs boson mass in GeV , obtained with $C L_{s}$.

| Mass (GeV) | Observed | Expected |
| :---: | :---: | :---: |
| 130 | 7.9 | 6.5 |
| 150 | 2.9 | 2.7 |
| 200 | 2.0 | 1.7 |
| 240 | 3.2 | 2.1 |
| 300 | 2.2 | 2.6 |
| 400 | 2.5 | 2.9 |
| 600 | 27.6 | 16.3 |



Figure 9: Expected (dashed) and observed (full line) 95\% CL upper limit on the SM Higgs boson production cross section as a function of the Higgs boson mass, expressed in multiples of the SM rate. Figures (a),(b),(c), (d) are different presentations of the same result.

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# Search for Charged Higgs Bosons in the $\tau+$ jets Final State in $t \bar{t}$ Decays with $1.03 \mathrm{fb}^{-1}$ of $p p$ Collision Data Recorded at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS Experiment 

The ATLAS Collaboration


#### Abstract

This note presents the results of a search for charged Higgs bosons, $H^{ \pm}$, in $1.03 \mathrm{fb}^{-1}$ of proton-proton collision data recorded at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS experiment at the LHC using the $\tau+$ jets channel in $t \bar{t}$ decays with a hadronically decaying $\tau$ lepton in the final state. The data agree with the Standard Model expectation leading to a limit on the product of branching ratios $\mathrm{BR}\left(t \rightarrow b H^{ \pm}\right) \times \mathrm{BR}\left(H^{ \pm} \rightarrow \tau v\right)$ of $0.03-0.10$ for $H^{ \pm}$masses in the range $90 \mathrm{GeV}<m_{H^{ \pm}}<160 \mathrm{GeV}$. In the context of the Minimal Supersymmetric Standard Model values of $\tan \beta$ larger than $22-30$ are excluded in the mass range $90 \mathrm{GeV}<m_{H^{ \pm}}<140 \mathrm{GeV}$.


## 1 Introduction

The charged Higgs boson is predicted by many non-minimal Higgs scenarios [1, 2], such as models containing Higgs triplets and Two-Higgs-Doublet Models (2HDM) [3]. The observation of charged Higgs bosons ${ }^{1}, H^{ \pm}$, would indicate physics beyond the Standard Model (SM). The analysis in this note considers the type II-2HDM [3], which is also the Higgs sector of the Minimal Supersymmetric Standard Model (MSSM) [4]. For charged Higgs boson masses, $m_{H^{+}}$, smaller than the top quark mass, $m_{t}$, the dominant production mode at the LHC for $H^{+}$is through top quark decay via $t \rightarrow H^{+} b$. The dominant source of top quarks at the LHC is through $t \bar{t}$ production; the cross section for charged Higgs boson production from top quark decays in single-top events is much smaller and not considered here. For $\tan \beta>3$, where $\tan \beta$ is the ratio of the vacuum expectation values of the two Higgs doublets, charged Higgs bosons decay mainly via $H^{+} \rightarrow \tau v$ [5]. Recent limits on light charged Higgs boson production come from the Tevatron [6], where the observed upper limit on $\operatorname{BR}\left(t \rightarrow H^{+} b\right)$ assuming $\operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)=1$ is 0.17 for $m_{H^{+}}=120 \mathrm{GeV}$. Direct searches at LEP [7] give a lower limit of $m_{H^{+}} \simeq 90 \mathrm{GeV}$ for $\operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)=1$. Preliminary results for charged Higgs boson searches in top quark decays have recently been made public by the CMS experiment [8].

This note describes the search for charged Higgs bosons in $t \bar{t}$ events in the topology shown in Fig. 1, for the case where both the $\tau$ lepton and the $W$ decay hadronically ( $\tau+\mathrm{jets}$ channel).

The $H^{+}$search uses proton-proton collision data collected with the ATLAS experiment [9] at the LHC at a center-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ in 2011. The total integrated luminosity amounts to $1.03 \mathrm{fb}^{-1}$.

The background processes that enter these searches include the production of $t \bar{t}$, single-top, $W+$ jets, $Z / \gamma^{*}+$ jets, and multi-jet events where there is either a true $\tau$ lepton, or another object misidentified as a hadronically decaying $\tau$. In this note, all significant backgrounds, i.e. events with correctly identified hadronically decaying $\tau$ leptons (hereafter referred to as $\tau$ jets), or with jets or electrons misreconstructed as $\tau$ jets, are estimated using data-driven methods.


Figure 1: Example for a leading-order Feynman diagram for the production of a charged Higgs boson through gluon fusion in $t \bar{t}$ decays.

## 2 Physics processes and their cross sections

All relevant backgrounds are estimated using data-driven techniques. However, for backgrounds with intrinsic missing transverse energy and objects misidentified as $\tau$ jets, simulation is used to model any aspects not related to the probability of the object to be misidentified as a $\tau$ jet. For backgrounds without

[^64]intrinsic $E_{\mathrm{T}}^{\text {miss }}$ (multi-jet background), simulation is used to subtract the electroweak and $t \bar{t}$ contribution in the control region. Simulation is also used for comparison with the results of the data-driven estimates.

The Monte Carlo (MC) simulation of $t \bar{t}$ and single-top events is based on MC@NLO [10] using HERWIG [11] for the hadronization process and JIMMY [12] for simulating multi-parton interactions. Overlap between $t \bar{t}$ and single-top final states is taken into account [13]. A $t \bar{t}$ production cross section of 165 pb [14] obtained from approximate NNLO calculations [15] is used (both for SM $t \bar{t}$ decays and decays via a charged Higgs boson). The MC@NLO cross sections are used for single-top production. Throughout this note, a top quark mass of 172.5 GeV is assumed.

ALPGEN [16] is used for the generation of $W+$ jets and $Z / \gamma^{*}+$ jets events with up to five partons from the hard matrix element, again together with HERWIG/JIMMY. The ALPGEN cross sections are rescaled by a factor $1.20(W)$ and $1.25\left(Z / \gamma^{*}\right)$ to match NNLO calculations [17]. The $H^{+}$signal events are generated with PYTHIA [18], using TAUOLA [19] for $\tau$ lepton decays and PHOTOS [20] for photon radiation off charged leptons. Event generators are tuned to describe ATLAS data, and the parameter sets AMBT1 [21] and AUET1 [22] are used for this purpose for events hadronized with Pythia, and with HERWIG/JIMMY, respectively.

Table 1: Simulated events used in this study. The $W / Z+$ jets as well as the $s$ - and $t$-channel single-top events are only simulated for decays involving leptons ( $\ell$ denotes $e, \mu$, or $\tau$ ), and the cross section given includes this branching ratio. The NLO+NNLL cross section is used for $t \bar{t}$, NLO for single-top, and NNLO for $W / Z+$ jets. The $H^{+}$sample uses $m_{H^{+}}=130 \mathrm{GeV}, \operatorname{BR}\left(t \rightarrow b H^{+}\right)=0.1$ and $\operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$ is assumed to be 1 .

| Process | Generator | Cross section [pb] |
| :--- | :--- | ---: |
| $t \bar{t}$ with $\geq 1 \ell$ | MC@NLO | 89.4 |
| single-top $(s, t, W t$ channel $)$ | MC@NLO | $21.4,1.41,14.6$ |
| $W \rightarrow \ell v+$ jets | ALPGEN | $3.1 \cdot 10^{4}$ |
| $Z / \gamma^{*} \rightarrow \ell \ell+$ jets | ALPGEN | $3.2 \cdot 10^{3}$ |
| $t \bar{t} \rightarrow b H^{ \pm} b W$ with $H^{ \pm} \rightarrow \tau v$ | PYTHIA | 29.6 |

All events are propagated through a detailed GEANT4 [23, 24] simulation of the ATLAS detector and reconstructed by the same algorithms as the data. Cross sections and simulated event samples are summarized in Table 1.

## 3 Object reconstruction

A description of the ATLAS detector can be found elsewhere [9]. In this section, the criteria used to identify and reconstruct physics objects such as leptons or jets are described.

Data quality: For both the $H^{+}$event selection and the data-driven background estimates, the following requirements are applied [25]: The sub-detectors relevant to the analyses have been operational, the LHC delivered stable beams, and there are no jets in the event consistent with coming from instrumental effects such as coherent noise in the electromagnetic calorimeter, or non-collision backgrounds. To further reject non-collision backgrounds, only events with a reconstructed primary vertex with at least five associated tracks are considered.

Jets: Jets are reconstructed with the anti- $k_{t}$ algorithm [26,27] with a size parameter value of $R=0.4$. The jet finder uses three-dimensional noise-suppressed clusters [28] in the calorimeter, reconstructed at
the electromagnetic (EM) energy scale. Jets are then calibrated to the hadronic energy scale with Monte-Carlo-based correction factors which depend on their transverse momentum ( $p_{\mathrm{T}}$ ) and pseudorapidity $(\eta)$. The jet energy scale uncertainty is estimated to be $(2.5-14) \%$, depending on $p_{\mathrm{T}}$ and $\eta$, with methods described in Ref. [29] but based on a larger data set. Jets considered in this analysis are required to have $p_{\mathrm{T}}>20 \mathrm{GeV}$ and $|\eta|<2.5$.
$\boldsymbol{b}$ jets: To identify jets initiated by $b$ quarks, a combination of a 3D-impact-parameter-based discriminant and a secondary-vertex-tagger [30] with an identification efficiency of about $60 \%$ for $b$ jets with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $t \bar{t}$ events is applied.
$\boldsymbol{\tau}$ jets: For the reconstruction of $\tau$ jets, all anti- $k_{t}$ jets in the calorimeter with $E_{\mathrm{T}}>10 \mathrm{GeV}$ are considered as $\tau$ candidates [31]. A dedicated algorithm is used to reject electrons (called tight electron veto). Only candidates with 1 or 3 associated tracks reconstructed in the inner detector are considered. Hadronic $\tau$ decays are identified using a likelihood quality criterion (corresponding to an efficiency of about $30 \%$ for $\tau$ leptons with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $Z \rightarrow \tau \tau$ events, and a rejection factor of about 100-1000 for quarkand gluon-initiated jets, depending on $p_{\mathrm{T}}, \eta$, and the number of associated tracks). For this analysis, they are required to have a visible $p_{\mathrm{T}}>20 \mathrm{GeV}$ and to be within $|\eta|<2.3$. In some control regions, a loose $\tau$ identification is used instead; this corresponds to an efficiency of $60 \%$, and a jet rejection of about 10 , depending on $p_{\mathrm{T}}$ and $\eta$.

Electrons: Electrons are reconstructed by matching clustered energy deposits in the electromagnetic calorimeter to tracks reconstructed in the inner detector [32]. They are required to meet quality requirements based on the expected shower shape of electrons [33]. Electrons are required to have $E_{\mathrm{T}}>20 \mathrm{GeV}$, and be isolated (defined by requiring less than 3.5 GeV of transverse energy - after corrections for pileup and leakage - in a cone of $\Delta R=0.2$ around the electron ${ }^{2}$, excluding the electron itself). Electrons are required to be in the fiducial volume of the detector, $|\eta|<2.47$. Electrons in the transition region $1.37<|\eta|<1.52$ are excluded.

Muons: Muon candidates are required to have a match of an inner detector track with a track reconstructed in the muon spectrometer [34]. Candidates are required to have $p_{\mathrm{T}}>10 \mathrm{GeV}$ and $|\eta|<2.5$. Only isolated muons are accepted by requiring that in a cone of $\Delta R=0.3$ around the muon (excluding the muon itself), both the energy deposited in the calorimeters and the momentum of all inner detector tracks total less than 4 GeV of transverse energy.

Missing transverse energy, transverse energy sum: The reconstructed missing transverse energy, $E_{\mathrm{T}}^{\text {miss }}$, is based on the energy deposited in the calorimeter and the momentum of tracks identified as associated to muons. Only noise-suppressed clusters of cells are used, and corrections for unclustered cells are applied. The contribution of the calorimeter cells is calibrated differently depending on which object they are associated to. For all jets, the same hadronic calibration scheme as for jet reconstruction is used while electrons are calibrated at the electromagnetic energy scale [35].

The transverse energy sum, $\sum E_{\mathrm{T}}$, is defined as the sum of the transverse energy of all the objects which have been reconstructed as detailed in this section, including missing transverse energy.

[^65]Overlap removal: When candidates selected using the above criteria overlap geometrically with one another (within $\Delta R<0.2$ ), this conflict is resolved by only selecting one candidate in the following order of priority: muon, electron, $\tau$ jet, or jet.

General systematic uncertainties The main detector-related systematic uncertainties are listed in Table 2. These are mostly related to identification efficiencies and the energy/momentum resolution and scale of the physics objects described above. Uncertainties on trigger efficiency, luminosity, cross sections and acceptance are also listed.

To assess the impact of most sources of systematic uncertainty on the result of the analysis, selection cuts for each analysis are re-applied after shifting a particular parameter by its $\pm 1$ standard deviation uncertainty. The luminosity and the trigger uncertainty with respect to the offline efficiency serve directly as scale factors on the event yield.

Table 2: Systematic uncertainties. Uncertainties on the $t \bar{t}$ cross section include variations of the parton density functions (pdf) and of the factorization and renormalisation scale. A scale factor is the ratio of efficiencies in data and simulation, and is here denoted as "SF". The difference in acceptance for $t \bar{t}$ events at LO and NLO is used as systematic uncertainty on the signal acceptance.

| Quantity | Uncertainty |
| :--- | :--- |
| Luminosity [36] | $\pm 3.7 \%$ |
| Jet energy resolution (JER) | $\pm(10-30) \%$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| Jet energy scale (JES) | $\pm(2.5-14) \%$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $E_{\mathrm{T}}^{\text {miss }}$ | Uncertainty due to scale/resolution uncertainties (e.g. JES); |
|  | additional $10 \%$ of pile-up-related uncertainty |
| $b$-tagging efficiency SF unc. | $\pm(0.05-0.15)$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $b$-tagging mistag rate | $\pm(0.16-0.39)$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $b$ jets JES uncertainty | an additional $\pm 2.5 \%$ on top of the standard JES |
| $\tau$ identification efficiency | $\pm(8.5-9.9) \%$, depending on $p_{\mathrm{T}}$ |
| $\tau$ energy scale | $\pm(4.5-6.5) \%$, depending on $p_{\mathrm{T}}, \eta$, number of associated tracks |
| $\tau$ electron mis-id correction factors | $\pm(23-100) \%$, depending on $\eta$; for one-prong only |
| $\tau+E_{\mathrm{T}}^{\text {miss trigger }}$ | $\pm 9 \%$ |
| $e$ reco. efficiency SF | $\pm(0.7-1.8) \%$, depending on $\eta$ |
| $e$ identification efficiency SF | $\pm(2.2-3.8) \%$, depending on $E_{\mathrm{T}}$ and $\eta$ |
| $e$ energy scale | $\pm(0.3-1.8) \%$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $e$ energy resolution | $\pm(0.5-2.4) \%$ (additional constant term), depending on $p_{\mathrm{T}}$ and $\eta$ |
| $\mu$ reco. efficiency SF | $\pm(0.25-0.55) \%$, depending on the data-taking period |
| $\mu$ momentum scale and resolution | $\pm(0.4-0.7) \%$, depending on $\eta$ |
| Initial/final state radiation modelling | $-16 \% /+19 \%(t \bar{\tau}$ signal and background) |
| Acceptance | $\pm 4 \%$ (background), $\pm 10 \%$ (signal) |
| $t \bar{t}$ cross section | $165_{-9}^{+4}($ scale $)+7($ pdf $)$ pb |

## 4 Event selection

This study describes the search for a charged Higgs boson in the topology

$$
\begin{equation*}
t \bar{t} \rightarrow\left[H^{+} b\right]\left[W^{-} \bar{b}\right] \rightarrow\left[\left(\tau_{h a d}^{+}+v\right) b\right]\left[\left(q \bar{q}^{\prime}\right) \bar{b}\right] \tag{1}
\end{equation*}
$$

where both the $W$ boson and the $\tau$ lepton decay hadronically. This topology has the advantage that the $W$ boson can be fully reconstructed, the $H^{+}$candidate can be reconstructed in the transverse plane, and
the branching ratio of the $W$ boson decay to quarks is larger than that to leptons; but it needs to be distinguished from a large multi-jet background.

The following selection cuts are applied, based on the reconstructed physics objects described in Section 3:

1. Event preselection:
(a) Data quality cuts.
(b) $E_{\mathrm{T}}^{\text {miss }}$ plus tau trigger $[37,38]$, with a threshold of 29 GeV on the $\tau$ object, of 35 GeV on $E_{\mathrm{T}}^{\text {miss }}$, and no muon corrections on $E_{\mathrm{T}}^{\text {miss }}$. The signal efficiency is about $70 \%$, depending on $m_{H^{+}}$.
(c) At least 4 jets (excluding $\tau$ jets) with $p_{\mathrm{T}}>20 \mathrm{GeV}$ and $|\eta|<2.5$.
2. A $\tau$ jet with $p_{\mathrm{T}}^{\tau}>35 \mathrm{GeV}$ within $|\eta|<2.3$ is required. This $\tau$ jet must be matched to the $\tau$ trigger object within $\Delta R<0.1$. Events with a second identified $\tau$ jet with $p_{\mathrm{T}}^{\tau}>20 \mathrm{GeV}$ are vetoed.
3. Events are vetoed if any identified electrons $\left(E_{\mathrm{T}}>20 \mathrm{GeV}\right)$ or muons $\left(p_{\mathrm{T}}>10 \mathrm{GeV}\right)$ are present.
4. The missing transverse energy $E_{\mathrm{T}}^{\mathrm{miss}}$ is required to be larger than 40 GeV .
5. Events with large reconstructed $E_{\mathrm{T}}^{\mathrm{miss}}$ due to the limited resolution of the energy measurement are rejected with a cut on the ratio $\frac{E_{\mathrm{T}}^{\text {miss }}}{0.5 \cdot \sqrt{\sum E_{\mathrm{T}}}}>8 \mathrm{GeV}^{1 / 2}$, using the $\sum E_{\mathrm{T}}$ definition described in Section 3. Considering the minimum $\sum E_{\mathrm{T}}$ required to pass all other selection cuts, this also corresponds to raising the cut on $E_{\mathrm{T}}^{\text {miss }}$ to about 50 GeV .
6. At least one $b$-tagged jet is required.
7. Topologies consistent with a top decay are identified by requiring that the $q q b$ candidate with the highest $p_{\mathrm{T}}^{q q b}$ value must satisfy $m(q q b) \in[120,240] \mathrm{GeV}$.

For events passing the above selection cuts the transverse mass, $m_{\mathrm{T}}$, is defined as

$$
\begin{equation*}
m_{\mathrm{T}}=\sqrt{2 p_{\mathrm{T}}^{\tau} E_{\mathrm{T}}^{\mathrm{miss}}(1-\cos \Delta \phi)} \tag{2}
\end{equation*}
$$

where $\Delta \phi$ is the azimuthal angle between the $\tau$ jet and the missing energy direction. This final discriminating variable is related to the $W$ boson mass in the $W \rightarrow \tau v$ background case, and the $H^{+}$mass for the signal hypothesis.

At the end of the selection cut flow, after applying data-driven methods as detailed in the sections that follow, $37 \pm 7$ background events are expected for $m_{\mathrm{T}}>40 \mathrm{GeV}$. Of those, $21 \pm 5$ events are expected with a correctly identified $\tau$ jet; about 2 events each for the case where an electron or a jet have been misidentified as a hadronically decaying $\tau$ lepton in a $t \bar{t}$ or electroweak background process. The multijet contribution is expected to be $12 \pm 5$ events. A potential signal yield depends on the charged Higgs boson mass and the branching ratio $t \rightarrow b H^{+}$; for example, 70 events are expected for $m_{H^{+}}=130 \mathrm{GeV}$ and $\operatorname{BR}\left(t \rightarrow b H^{+}\right)=0.1$.

## 5 Data-driven background estimation

The main source of background events to charged Higgs boson searches at the LHC are those coming from production processes such as $t \bar{t}$, multi-jet, single top-quark, and $W+$ jets, in this order of relevance. The individual contributions from these backgrounds are determined in a data-driven way. They can
be divided into two categories: backgrounds with intrinsic $E_{\mathrm{T}}^{\text {miss }}$ from $W$ decays, and backgrounds with $E_{\mathrm{T}}^{\text {miss }}$ caused by detector effects (multi-jet events). For the first category, the contribution from events in which electrons or jets are misidentified as $\tau$ jets are predicted using appropriate control samples while events with correctly identified $\tau$ jets are studied with the embedding method. The multi-jet background can be estimated using the shape of its $E_{\mathrm{T}}^{\text {miss }}$ distribution in a suitable control region.

### 5.1 Methods based on measuring misidentification probabilities

The background from events where an electron or a jet is misidentified as a hadronically decaying $\tau$ lepton is estimated in a data-driven procedure from suitable control samples. The probability for an electron or jet to be misidentified as a $\tau$ jet is defined as
misidentification probability $=\frac{\text { number of } \tau \text { candidates passing event selection, } \tau \text { ID and electron veto }}{\text { number of } \tau \text { candidates passing event selection }}$.

### 5.1.1 Electron-to- $\tau$ misidentification probability with a tag-and-probe method

The Method A tag-and-probe method on $Z / \gamma^{*}$ events in collision data is used to measure the misidentification probability of electrons. The result is compared to simulation, and the ratio of the misidentification probability as measured in data to that determined in simulation is called a scale factor. This factor is then used to correct the description of the electron-to- $\tau$ misidentification probability in simulation. The method used is identical to that described in [39] though based on a larger data set. The process $Z / \gamma^{*} \rightarrow e e$ allows the selection of a clean sample of electrons from data. An electron trigger with a threshold on the electron $E_{\mathrm{T}}$ of 20 GeV is used. The tag electron is required to have a $p_{\mathrm{T}}>30 \mathrm{GeV}$ and to be located in the central region $(|\eta|<2.47)$ of the detector (but outside the transition region between the barrel and the end-cap, $1.37<|\eta|<1.52$ ). It must be isolated (the sum of the momenta of tracks in a cone of $\Delta R=0.4$ around the electron is required to be less than $6 \%$ of the electron momentum) and must pass tight electron identification criteria [33]. Furthermore, a match within $\Delta R=0.1$ to the trigger electron is required. The probe electron is considered for further analysis if it is reconstructed as a $\tau$ jet candidate with $p_{\mathrm{T}}>20 \mathrm{GeV}$ with exactly one associated track. The probability of electrons to be misidentified as 3-track $\tau$ jets is negligible. The pair with the highest scalar $E_{\mathrm{T}}$ sum is chosen from all possible $e-\tau$ pairs that are separated by $\Delta R>0.4$. Additionally, the tag and the probe objects are required to have opposite electric charges. Events with $E_{\mathrm{T}}^{\text {miss }}>20 \mathrm{GeV}$ are discarded to reduce the background contamination from $W \rightarrow e v$ decays, and the invariant mass of the $e-\tau$ pair is required to be between 80 and 100 GeV .

The selected probe sample of $\tau$ jet candidates then contains electrons originating from $Z$ bosons with a purity (estimated from simulation) of about $99 \%$. The main backgrounds are multi-jet events, $W \rightarrow e v$, and $Z / \gamma^{*} \rightarrow \tau \tau$, in that order. The multi-jet background is estimated using a two-dimensional sideband subtraction method [39], the electroweak backgrounds using simulation.

Results The misidentification probabilities (as defined in Eq. 3) are extracted for the $\tau$ candidates which pass the $\tau$ selection (including overlap removal with electron candidates) and the electron veto criteria as used in the $H^{+}$selection. In the denominator, the probe objects are not required to pass the $\tau$ jet identification, whereas the numerator contains the number of events with the probe objects both passing the identification and not being discarded by the electron veto. The results for the scale factor and misidentification probability are shown in Table 3 for the different calorimeter regions. Only the scale factors are used in the following. No significant dependence of the scale factor on the $p_{\mathrm{T}}$ of the $\tau$ lepton candidate is observed.

Application of the method to estimate the $e \rightarrow \tau$ misidentification background The misidentification probability from this study is applied by scaling simulated events in which the selected reconstructed $\tau$ jet originates from a true electron. The scale factor used is given by the ratio of the misidentification probability in data to that in Monte Carlo.

Table 3: Scale factors and measured $e \rightarrow \tau$ misidentification probabilities for $\tau$ candidates with $E_{\mathrm{T}}>20$ GeV in the barrel $(0<|\eta|<1.37)$, transition $(1.37<|\eta|<1.52)$ and end-cap $(1.52<|\eta|<2.5)$ regions passing the $\tau$ identification and a tight electron veto, for a $\tau$ identification efficiency of about $30 \%$. The scale factors are given with statistical and systematic uncertainties combined.

| Region | Scale factor | Misidentification probability (data) |
| :--- | ---: | ---: |
| $0<\|\eta\|<1.37$ | $1.1 \pm 0.3$ | $0.0028 \pm 0.0006$ |
| $1.37<\|\eta\|<1.52$ | $1.0 \pm 1.0$ | $0.0005 \pm 0.0004$ |
| $1.52<\|\eta\|<2.5$ | $1.6 \pm 0.5$ | $0.009 \pm 0.003$ |

Systematic uncertainties Five main sources of systematic uncertainties on the electron- $\tau$ jet misidentification probability are studied. The systematic uncertainty due to the subtraction of multi-jet and electroweak backgrounds is at the level of only $1 \%$, but can reach up to $25 \%$ in the transition region. Ideally, the measurement should be independent of the tag selection. To test any potential correlation, this selection has been varied (using medium electron identification criteria instead of tight ones in order to study the bias of only selecting very well-reconstructed tag electrons), leading to an estimate of a systematic uncertainty of $10 \%$. Other systematic uncertainties are negligible in comparison. The choice of the mass window size around $m_{Z}$ applied to the tag-and-probe objects which could result in a bias by only studying objects with well-reconstructed momentum and the uncertainty of the electron energy scale (via the cut on the tag electron energy) only give a small contribution. The total uncertainties on the scale factors (combining the statistical and systematic uncertainties of the measurement) are $24 \%$ in the barrel, $29 \%$ in the end-caps, and $100 \%$ in the transition region. Except for the end-cap, they are dominated by the statistical uncertainties.

In total, the expected contribution of events with electrons misidentified as $\tau$ jets in the signal region is about 2 events which is about $5 \%$ of the expected background. Thus reducing the relatively large uncertainties would only lead to a minor improvement of the $H^{+}$sensitivity.

### 5.1.2 Jet-to- $\tau$ misidentification probability from photon+jets

To study the probability for jets to be misidentified as hadronically decaying $\tau$ leptons, a $\gamma$-jet control sample is used. Like jets from the hard process in the dominant $H^{+}$background $t \bar{t}$, jets in this control sample originate predominantly from quarks as opposed to gluons. A measurement of the probability for a jet to be misidentified as a hadronically decaying $\tau$ lepton is performed using $1.03 \mathrm{fb}^{-1}$ of data and is used to predict the yield of jet-to- $\tau$ misidentification events from the most important SM backgrounds with intrinsic $E_{\mathrm{T}}^{\text {miss }}$. The main difference between $t \bar{t}$ and $\gamma$-jet events is the different fraction of $b$ jets which is smaller in $\gamma$-jet events. However, the probability for a $b$ jet to be misidentified as a $\tau$ jet is smaller than the corresponding probability for a light-quark jet: The average track multiplicity of $b$ jets is higher, and variables which measure the mass of the $\tau$ candidate allow a good discrimination. Hence using the $\gamma$-jet misidentification probability leads to a higher background estimate and is thus conservative.


Figure 2: Jet $\rightarrow \tau$ misidentification probability measured from $\gamma$-jet events for jets with 1 or 3 associated tracks as a function of $p_{\mathrm{T}}$ and $\eta$. The error bars indicate the size of the statistical uncertainties.

The Method Events are required to pass a single-photon trigger (with an $E_{\mathrm{T}}$ threshold of 15,20 or 40 GeV ). The photon candidate must be isolated (less than 6 GeV of $E_{\mathrm{T}}$ deposited in a $\Delta R=0.2$ cone around the photon), is required to match a trigger object, pass the photon selection [40], and have either zero or two associated tracks to include photon conversions. The photon candidate must have $|\eta|<2.37$, not be located in the transition region, and must have a transverse energy of at least 15 GeV . The selected $\gamma$-jet sample consists of events with one photon candidate and a jet with $p_{\mathrm{T}} \geq 20 \mathrm{GeV}$, separated in $\phi$ by at least 2.84 radians. The difference in transverse energy between the jet and the photon must be less than half of the total transverse energy of the photon. Any additional jets are required to have less than $20 \%$ of the photon transverse energy.

The misidentification probability is measured as a function of both $p_{\mathrm{T}}$ and $\eta$. The denominator of the calculated misidentification probability is the number of events with a $\tau$ candidate (i.e. no $\tau$ ID applied) with $p_{\mathrm{T}}$ greater than 20 GeV and $|\eta|<2.3$, which passes an electron veto. The misidentification probability is evaluated separately for the case of candidates with 1 or 3 associated tracks. Among all jets with $E_{\mathrm{T}}>20 \mathrm{GeV}$ and $|\eta|<2.3$, the fraction of light-quark jets which are considered as such $\tau$ candidates is about $27 \%$. The numerator in the calculated misidentification probability consists of events with objects which pass the full $\tau$ identification. They must not be within $\Delta R=0.2$ of any $e$ or $\mu$. The measured misidentification probabilities are shown in Fig. 2.

Systematic uncertainties The dominant systematic uncertainties on the misidentification probability are (the ranges given on each systematic uncertainty show the variation with the $p_{\mathrm{T}}$ and $\eta$ of the $\tau$ candidate):

- Contamination of the control sample with true $\tau$ jets from $Z \rightarrow \tau \tau$ and $W \rightarrow \tau v$ events, evaluated using simulation: $(1-3) \%$.
- Contamination of the control sample with multi-jet events which have a larger gluon-initiated jet fraction than $\gamma$-jet events. The associated systematic uncertainty is evaluated by modifying the photon ID requirements, in particular loosening the photon isolation which increases the impurity from multi-jet events in the control sample: $(5-9) \%$.
- Contamination of the control sample by three-jet events. The associated systematic uncertainty is evaluated by varying the selection cuts (vetoing events with additional jets with less than 0.1 of the
photon momentum), and by splitting the control sample in a part which fulfills even tighter requirements and one which does not, and then taking the variation of the misidentification probability due to these changes as the uncertainty: $(11-17) \%$.
- The measurement of the misidentification probability on the probe object is assumed to be uncorrelated from the selection of the tag object. To evaluate uncertainties from a violation of this assumption, correlations between the tag and the probe objects are studied by changing the requirements on the tag object (requiring a photon with a looser quality criterion) and studying the impact on the measurement of the misidentification probability on the probe object: $(7-14) \%$.

Additionally, the statistical uncertainty of the measurement of the misidentification probability enters as uncertainty on any application of the misidentification probability. The total systematic uncertainty is about $(15-24) \%$, depending on $p_{\mathrm{T}}$ and $\eta$. The systematic uncertainties on the misidentification probability are propagated into the background prediction for the baseline selection and enter the statistical evaluation as shape uncertainties.

Application to estimate the jet $\rightarrow \tau$ misidentification background To predict the background in $\mathrm{H}^{+}$ searches, the measured jet $\rightarrow \tau$ misidentification probability is applied to simulated $t \bar{t}$, single-top, and $W+$ jets events. These events are required to pass the full event selection except for the $\tau$ identification. For these events, $\tau$ candidates fulfilling the same requirements as in the misidentification probability definition which do not overlap with a true $\tau$ lepton are identified. Out of the remaining $\tau$ candidates, each one is considered to be potentially misidentified as a $\tau$ jet separately. The identified jet that corresponds to the $\tau$ candidate is removed from the event, affecting the number of reconstructed jets, the $E_{\mathrm{T}}^{\text {miss }}$ significance of the event, and the number of $b$-tagged jets. If, after taking this into consideration, the event still passes the selection, then the event is counted as background event with a weight given by the misidentification probability corresponding to the $p_{\mathrm{T}}$ and the $\eta$ of the $\tau$ candidate. The predicted number of events from the $t \bar{t}$ sample, together with a comparison to the MC prediction using truth information, is shown in Table 4. All other jet $\rightarrow \tau$ misidentification backgrounds with intrinsic $E_{\mathrm{T}}^{\text {miss }}$ are at least two orders of magnitude smaller than $t \bar{t}$.

Table 4: Application of the misidentification probability obtained from $\gamma$-jet events. The numbers shown are the expected number of events in collision data after the $H^{+}$selection. The prediction based on the misidentification probability measurement (statistical and systematic uncertainties), as well as the MC prediction (statistical uncertainties), are given.

| Sample | Data-driven prediction [number of events] | MC prediction [number of events] |
| :--- | :--- | :--- |
| $t \bar{t}$ | $2.8 \pm 1.0($ stat $) \pm 0.5($ syst $)$ | $3.8 \pm 0.6($ stat $)$ |

### 5.2 Multi-jet background estimate

As the uncertainties on the multi-jet expectation are large, it is necessary to avoid using any multi-jet simulation to estimate this background. Thus an approach different from estimating the jet $\rightarrow \tau$ misidentification contribution in events with intrinsic $E_{\mathrm{T}}^{\text {miss }}$, as described in the previous section, is chosen.

The Method The multi-jet background is estimated by fitting its $E_{\mathrm{T}}^{\text {miss }}$ shape (and the $E_{\mathrm{T}}^{\text {miss }}$ shape of other backgrounds) to data. In order to study this shape in a data-driven way, a control region is defined
where the $\tau$ identification and $b$-tagging requirements are inverted. The $\tau$ candidates must pass a loose $\tau$ identification but fail the tight $\tau$ identification used in the baseline selection. In addition, the event is required not to contain any $b$-tagged jets and therefore also the requirement on the $q q b$ mass (selection cut 7) is removed.

Assuming that the shapes of the $E_{\mathrm{T}}^{\text {miss }}$ and $m_{\mathrm{T}}$ distributions are the same in the control sample and signal regions (see Fig. 3 for a comparison early in the selection cut flow), the shape of the $E_{\mathrm{T}}^{\text {miss }}$ distribution is used to model the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution for the multi-jet background (after subtracting the background from other processes). The $E_{\mathrm{T}}^{\text {miss }}$ distribution measured in data (for the baseline selection) is then fitted using two shapes: this multi-jet model, and the sum of other processes (dominated by $t \bar{t}, W+\mathrm{jets}$ ) for which the shape and the relative normalisation are taken from MC simulation. The free parameters in the fit are the overall normalisation (to the one in data) and the multi-jet fraction.


Figure 3: Distribution of $E_{\mathrm{T}}^{\text {miss }}$, after subtracting the expectation from $t \bar{t}, W+\mathrm{jets}$, and single-top simulation; compared are the distributions after requirement 3 of the baseline selection as detailed in Section 4, with the exception that in the control region, the $\tau$ selection and the $b$-tagging requirements have been inverted. The shaded area indicates the size of the statistical uncertainties.

Systematic uncertainties The dominant systematic uncertainties are:

- The uncertainty on the assumption that the $E_{\mathrm{T}}^{\mathrm{miss}}$ shape is identical in the signal and control regions. This is studied by varying the number of entries in each bin separately within the maximum differences observed early in the selection cut flow (a factor of 0.5 and 2.0) and redoing the fit. Then, the largest downwards and upwards fluctuations are used as systematic uncertainty. This leads to an uncertainty on the multi-jet fraction of $-13 \% /+25 \%$.
- The uncertainty on the $t \bar{t}$ and $W+$ jets shapes and relative normalisation from Monte Carlo is dominated by uncertainties on the $t \bar{t}$ cross section. The scaling of the $t \bar{t}$ Monte Carlo is varied according to these uncertainties, leading to an uncertainty on the multi-jet fraction of $2.4 \%$.
- The uncertainty from backgrounds other than $t \bar{t}$ and $W+$ jets in the control region is found to be negligible.

The uncertainty on the multi-jet fraction is dominated by the statistical uncertainty of the data set on which the fit is performed.

Result of the data-driven estimate of the multi-jet background The multi-jet fraction is estimated to be $(23 \pm 10) \%$ using the fit to the $E_{\mathrm{T}}^{\text {miss }}$ distribution shown in Fig. 4. The $m_{\mathrm{T}}$ distribution for the same
events is shown in Fig. 5. Except for the multi-jet background, all other processes have $W$ bosons in the final state and their distributions drop off around the $W$ boson mass, as expected. Such behavior is neither expected nor observed for the multi-jet background as resulting shapes are mainly caused by detector effects. To probe the region with large $m_{\mathrm{T}}$, in which a potential $H^{+}$signal resides, it is thus important to suppress the multi-jet background as much as possible.


Figure 4: Multi-jet estimate: A fit to the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution in data after all selection cuts using two shapes (one for the multi-jet model, and one for all other background processes, dominated by $t \bar{t}$ and $W+$ jets) is shown. The multi-jet fraction estimated after all selection cuts is $(23 \pm 10) \%$.


Figure 5: Contribution of multi-jet events to the $m_{\mathrm{T}}$ distribution after all cuts of the $H^{+}$selection. The multi-jet fraction is estimated using the fit to the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution shown in Fig. 4.

### 5.3 Embedding method

Complementary to the methods based on misidentification probability, an embedding method is used for estimating the background from true $\tau$ jets, described below. The method consists of collecting a control sample of $t \bar{t}$, single-top, and $W+$ jets events with a muon in data, and replacing the detector signature of this muon with that of a simulated $\tau$ lepton. The reconstruction is re-applied to the new hybrid
events which are then used to estimate the background to the $H^{+}$selection. The advantage is that the whole event (except for the $\tau$ jet) is taken directly from data, including the underlying event and pile-up, missing energy, $b$-quark jets and light-quark jets. The method has been validated in $\tau+$ jets events using early ATLAS data [41].

### 5.3.1 The Method

Control sample selection To select the $t \bar{t}$-like $\mu+$ jets control sample from data, the following event selection is used:

- Event triggered by a single muon trigger ( $p_{\mathrm{T}}$ threshold of 18 GeV ),
- data quality cuts as described in Section 3,
- exactly one isolated muon with $p_{\mathrm{T}}>25 \mathrm{GeV}$,
- no isolated electron with $p_{\mathrm{T}}>20 \mathrm{GeV}$,
- at least four jets with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $|\eta|<2.5$,
- at least one of the jets is $b$-tagged (nominal efficiency of $65 \%$ ),
- missing transverse energy $E_{\mathrm{T}}^{\text {miss }}>30 \mathrm{GeV}$,
- scalar sum of energy of reconstructed objects $\sum E_{\mathrm{T}}>200 \mathrm{GeV}$.

This selection is looser than the selection defined in Section 4 in order not to bias the control sample. This also applies to the $\tau$ jet which carries the momentum of the selected muon minus the momentum of the neutrino in the $\tau$ lepton decay and its $p_{\mathrm{T}}$ is required to be larger than 35 GeV in the $H^{+}$selection. The impurity from the background with muons produced in $\tau$ decays, and non-isolated muons (dominantly $b \bar{b}$ and $c \bar{c}$ events) is at the level of $10 \%$ and biases the shape of embedded events. However, the bias is greatly reduced as these events are much less likely to pass the $H^{+}$selection.

Embedding step After events have been selected, the actual embedding step takes place. The muon in the event is selected and its vertex position and momentum are extracted. The momentum is then rescaled to account for the higher $\tau$ lepton mass and fed into TAUOLA to produce the $\tau$ lepton decay products and generate final state radiation. The result is propagated through ATLAS detector simulation, followed by reconstruction. In the next step, tracks, calorimeter deposits and segments in the muon spectrometer in the vicinity of the muon are replaced with those of the simulated $\tau$ lepton decay products.

Comparison of embedding method versus simulation To test the method, the embedded data events are compared to simulated $t \bar{t}$ events (hereafter referred to as 'reference') in which the $\tau$ lepton comes directly from simulation of the whole event, and is not added via the embedding method. To make sure the set of events is comparable, both for the embedded and the reference events, a reconstructed $\tau$ candidate which is matched to a true $\tau$ lepton is required (this can be performed using embedded events, as the $\tau$ part of the event is taken from simulation).

A comparison of distributions of variables relevant to this analysis is shown in Fig. 6. A good agreement is observed within the statistical uncertainties.


Figure 6: Validation plots for the embedding method used to estimate the background with true $\tau$ jets. Embedded data is compared to $t \bar{\tau}$ simulation after applying the $H^{+}$selection. The $\tau$ likelihood (TauLLH), the $\tau$ transverse momentum, the missing transverse energy, and the top quark transverse momentum on the $t \rightarrow b q q$ side are shown. The plots are normalized to unit area. The shaded area indicates the size of the statistical uncertainties on the MC simulation.

### 5.3.2 Application to estimate the true- $\tau$ background

The contribution of backgrounds with true $\tau$ jets to the final $m_{\mathrm{T}}$ distribution is estimated from this distribution for embedded events. The normalisation is taken from collision data events in the region $0-40 \mathrm{GeV}$ of this distribution, where any signal contamination would be low for the expected range of sensitivity $\left(\operatorname{BR}\left(t \rightarrow b H^{+} \approx 5 \%\right)\right)$. Such a contamination is dealt with in the limit-setting process by subtracting the expected signal from the observed data before normalizing the shape to the region $m_{\mathrm{T}}<40 \mathrm{GeV}$. This is done when evaluating the signal+background hypothesis and takes the tested $\mathrm{BR}\left(t \rightarrow b H^{+}\right)$into account. Effectively, this brings the signal+background expectation closer to the background-only expectation.

The following procedure is applied:

1. Apply the $\tau+$ jets event selection to embedded events to obtain the $m_{\mathrm{T}}$ shape.
2. From collision data, count the number of events in the $m_{\mathrm{T}}$ distribution between $0-40 \mathrm{GeV}$ after subtracting the background from objects misidentified as $\tau$ jets.
3. Using this number, normalize the $m_{\mathrm{T}}$ distribution from embedded events using the ratio of events in collision data and embedded data.

For technical reasons, the trigger simulation cannot be re-run for embedded events. As the number of events entering the embedding control sample and passing the whole event selection is still relatively small, the event selection applied to the embedded events is modified by requiring a $\tau$ identified using loose criteria. This can be done because the $m_{\mathrm{T}}$ distribution is normalized to data and, as Fig. 7 (left) shows, the looser cuts do not bias the shape significantly.

The result is shown in Fig. 7 (right). As can be seen, the uncertainty of the background estimate is currently limited by the statistical uncertainty due to the limited number of events in the $t \bar{t}$ control sample. In the range $40<m_{\mathrm{T}}<300 \mathrm{GeV}$, there are $21 \pm 5$ background events with true $\tau$ jets expected where the uncertainty is due to the limited number of events in the control sample, and of the data in the region to which the shape is normalized to. In data, 26 events are observed after subtracting the background predicted by the misidentification probability methods and the multi-jet estimate. Within statistical uncertainties, the background prediction and data agree well.

### 5.3.3 Systematic uncertainties

The following systematic uncertainties are associated with the background prediction:

- To study the effect of additional multi-jet background on the embedding and the control sample selection itself, the $\mu$ isolation requirement is varied. To study a potential bias introduced by the embedding method parameters chosen, alternative values are used for the inner and outer cone size in which calorimeter cell depositions are replaced or added. To account for the fact that a small amount of pile-up-related activity can be present in the calorimeter cells removed in a cone around the muon, the effect of only removing half of this energy before adding the $\tau$ jet is studied. This results in a systematic uncertainty of $7 \%$ on the background normalisation.
- The systematic uncertainty due to the difference in the $m_{\mathrm{T}}$ shape as a consequence of loosening the selection with respect to the $H^{+}$selection, as shown in Fig. 7, results in a $8 \%$ uncertainty on the background normalisation, and a shift of about 2 GeV in the $m_{\mathrm{T}}$ distribution.
- The impact of the incomplete treatment of the $\tau$ polarisation in embedded events results in an uncertainty on the $m_{\mathrm{T}}$ shape which is estimated by comparing bin by bin the difference in the number of events for simulated $t \bar{t}$ events with and without correct treatment of the $\tau$ polarisation.


Figure 7: Left: Comparison of the $m_{\mathrm{T}}$ shape for simulation and for embedded events (with loose $\tau$ identification) used to estimate the background with true $\tau$ jets. The distribution from simulation is shown both after the $H^{+}$baseline selection and after the same selection but without trigger requirement and loose $\tau$ identification. All distributions are normalized to unit area. Right: Comparison of the $m_{\mathrm{T}}$ shape for embedded events versus collision data. The prediction using the embedding method is stacked on top of the expected backgrounds with objects misidentified as $\tau$ jets: MC expectation for $t \bar{t}$ and electroweak processes, and the data-driven estimate for multi-jet events. The comparison is done after the $H^{+}$event selection and after normalizing the $m_{\mathrm{T}}$ distribution of embedded events to the data distribution in the range $0-40 \mathrm{GeV}$. The gray area indicates the size of the statistical and systematic uncertainties of the embedding method estimate.

This results in an uncertainty on the normalisation of $15 \%$, and the $m_{\mathrm{T}}$ distribution is shifted by about 7 GeV which corresponds to $14 \%$ of the average $m_{\mathrm{T}}$.

- The impact on the $m_{\mathrm{T}}$ distribution due to the uncertainty on the $\tau$ energy scale (Table 2 ) is evaluated, leading to a normalisation uncertainty of $+4 /-2 \%$, and a shift in the $m_{\mathrm{T}}$ distribution by $\pm 1 \mathrm{GeV}$.

The statistical uncertainty of the estimate is $8 \%$ due to the limited size of the control sample, and additionally $20 \%$ due to the normalisation to data (allowing data to fluctuate within one standard deviation for $m_{\mathrm{T}}<40 \mathrm{GeV}$ ). The numbers above are only indicative, for the limit calculation the full shape uncertainty is used.

## 6 Results

The results of the data-driven methods in estimating the contributions of the various categories of backgrounds after the baseline selection are summarized in Table 5, and the $m_{\mathrm{T}}$ distribution of the remaining events is shown in Fig. 8. The total systematic uncertainty on the background prediction is about $30 \%$ but can reach up to $70 \%$ for $m_{\mathrm{T}}>100 \mathrm{GeV}$. For the signal, the total systematic uncertainty on the yield is about $40 \%$ with a small dependence on $m_{H^{+}}$. The number of events with true $\tau$ jets has been estimated with the embedding method, the jet $\rightarrow \tau$ misidentification events with intrinsic $E_{\mathrm{T}}^{\text {miss }}$ with $\gamma+\mathrm{jets}$ control samples, the $e \rightarrow \tau$ misidentification events with $Z / \gamma^{*} \rightarrow e e$ control samples, and the multi-jet contribution by taking its shape from a sideband region and fitting it to the data. The number of events with $m_{\mathrm{T}}>40 \mathrm{GeV}$ is given which allows for a better comparison of data and expectation as the estimate from the embedding method is normalized to data in the range $m_{\mathrm{T}}<40 \mathrm{GeV}$. A good agreement between the estimated and the observed number of events is seen.

Table 5: Expected number of events from data-driven estimates with $m_{\mathrm{T}}>40 \mathrm{GeV}$, and as observed in data. Only statistical uncertainties are given.

|  | Events with/from |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | true $\tau$ jets | jet $\rightarrow \tau$ mis-id | $e \rightarrow \tau$ mis-id | multi-jet | expected (sum) | data |
| $m_{\mathrm{T}}>40 \mathrm{GeV}$ | $21 \pm 5$ | $2.4 \pm 0.7$ | $1.9 \pm 0.2$ | $12 \pm 5$ | $37 \pm 7$ | 43 |

Using data-driven background estimates, no statistically significant excess of events is observed in $1.03 \mathrm{fb}^{-1}$ of collision data. Exclusion limits are set on the branching ratio $t \rightarrow b H^{+}$, and in the $m_{H^{+}}-\tan \beta$ plane, by rejecting the signal hypothesis at the $95 \%$ confidence level applying the $\mathrm{CL}_{s}$ procedure [42, 43]. A profile likelihood ratio [44] is used with the $m_{\mathrm{T}}$ distribution as the discriminating variable. The statistical analysis is based on a binned likelihood function for the $m_{\mathrm{T}}$ distribution. Systematic uncertainties in shape and normalisation are incorporated via nuisance parameters and the one-sided profile likelihood ratio, $\tilde{q}_{\mu}$, is used as a test statistic. The final limits are based on the asymptotic distribution of the test statistic [44].

The resulting exclusion limit is shown in Fig. 9 in terms of $\operatorname{BR}\left(t \rightarrow H^{+} b\right) \times \operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$. Figure 10 shows the upper limit in the context of the $m_{h}^{\max }$ scenario of the MSSM [45] in the $m_{H^{+-}} \tan \beta$ plane. No exclusion limit is shown for charged Higgs boson masses close to 160 GeV as no reliable calculations for $\mathrm{BR}\left(t \rightarrow H^{+} b\right)$ exist for $\tan \beta$ values in the range of interest. The following relative uncertainties on $\mathrm{BR}\left(t \rightarrow b H^{+}\right)$are considered [46]: 5\% for one-loop electro-weak corrections missing in the calculations, $2 \%$ for missing two-loop QCD corrections, and about $1 \%$ (depending on $\tan \beta$ ) $\Delta_{b^{-}}$ induced uncertainties (where $\Delta_{b}$ is a correction factor to the running bottom quark mass [47]). These


Figure 8: The $m_{\mathrm{T}}$ distribution after event selection. The observation in collision data, and the estimates from data-driven methods are compared. The distribution of the $H^{+}$signal is given for a reference point in parameter space corresponding to $\mathrm{BR}\left(t \rightarrow b H^{+}\right)=10 \%$, thus the SM-like $t \bar{t}$ background is reduced correspondingly.
uncertainties are added linearly. This result constitutes a significant improvement compared to existing limits provided by the Tevatron experiments [6] over the whole investigated mass range, but in particular for charged Higgs boson masses close to the top quark mass.

## 7 Conclusions

Charged Higgs bosons are searched for in the decay mode $t \rightarrow b H^{+}, H^{+} \rightarrow \tau v$, with hadronically decaying $\tau$ leptons, using $t \bar{t}$ events reconstructed in a total of $1.03 \mathrm{fb}^{-1}$ of $\sqrt{s}=7 \mathrm{TeV} p p$ collision data recorded with the ATLAS experiment. Data-driven methods, employed to estimate the number of background events characterized by the presence of a $\tau$ jet, $E_{\mathrm{T}}^{\text {miss }}, b$ jets, and a hadronically decaying $W$ boson, predict $37 \pm 7$ (stat) events with $m_{\mathrm{T}}>40 \mathrm{GeV}$. A total of 43 such events are observed which is consistent with the prediction. The $\mathrm{CL}_{s}$ procedure is used to derive $95 \%$ CL exclusion limits. Values of the product of branching ratios, $\mathrm{BR}\left(t \rightarrow b H^{+}\right) \times \mathrm{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$, larger than $0.03-0.10$ have been excluded in the $H^{+}$mass range $90-160 \mathrm{GeV}$, significantly extending limits from other experiments. Interpreted in the context of the $m_{h}^{\max }$ scenario of the MSSM, values of $\tan \beta$ above $22-30$ (depending on $m_{H^{+}}$) can be excluded in the mass range $90 \mathrm{GeV}<m_{H^{ \pm}}<140 \mathrm{GeV}$.

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Figure 9: Expected and observed $95 \%$ CL exclusion limits for charged Higgs boson production from top quark decays as a function of $m_{H^{+}}$in terms of $\mathrm{BR}\left(t \rightarrow H^{+} b\right) \times \mathrm{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$. For comparison, the best limit provided by the Tevatron experiments is shown [6].


Figure 10: Limit for charged Higgs boson production from top quark decays in the $m_{H^{+-}} \tan \beta$ plane. Results are shown for the MSSM scenario $m_{h}^{\max }$.
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## A Limit figure with PCL



Figure 11: Expected and observed $95 \%$ CL exclusion limits for charged Higgs boson production from top quark decays as a function of $m_{H^{+}}$in terms of $\mathrm{BR}\left(t \rightarrow H^{+} b\right) \times \mathrm{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$ using the $\mathrm{CL}_{s}$ procedure. Power-Constrained limits (PCL) [48] with a $50 \%$ power constraint are shown as well. For comparison, the best limit provided by the Tevatron experiments is shown [6].

## ATLAS NOTE

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# Search for the Standard Model Higgs boson in the diphoton decay channel with $4.9 \mathbf{f b}^{-1}$ of ATLAS data at $\sqrt{s}=7 \mathbf{~ T e V}$ 

The ATLAS collaboration


#### Abstract

This note presents a search for the Standard Model Higgs boson in the diphoton decay channel in proton-proton collisions at a centre-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ using data corresponding to an integrated luminosity of $4.9 \mathrm{fb}^{-1}$ collected with the ATLAS detector at the LHC. Over the diphoton mass range $110-150 \mathrm{GeV}$ the maximum deviation from the background-only expectation is observed at 126 GeV with a local significance of 2.8 standard deviations. Taking the look-elsewhere effect into account, the significance is 1.5 standard deviations. The expected cross section exclusion at $95 \%$ confidence level varies between 1.6 and 2.9 times the Standard Model cross section over the mass range 110150 GeV . The observed exclusions lie between 0.9 and 4.0 times the Standard Model cross section, and a Standard Model Higgs boson is excluded at $95 \%$ confidence level in the mass range of $114-115 \mathrm{GeV}$ and $135-136 \mathrm{GeV}$.


## 1 Introduction

The low mass region, in which the Standard Model (SM) Higgs boson [1-3] is not yet excluded, is constrained from below at 114.4 GeV by the LEP experiments [4] and from above at 141 GeV by the ATLAS and CMS experiments [5]. The diphoton decay mode is one of the most important channels in the search for the Higgs boson in this region. This note presents the search for the Higgs boson in the diphoton decay channel with an integrated luminosity of $4.9 \mathrm{fb}^{-1}$, corresponding to the total protonproton collision data sample recorded with the ATLAS detector [6] in 2011 at a centre-of-mass energy of 7 TeV . The general analysis strategy closely follows the one described in Ref. [7], but some refinements have been introduced to the categorization of events, as described below.

This note is organized as follows. The photon reconstruction and event selection are described in Section 2. The event categorization is illustrated in Section 3, and the signal and background modelling are discussed in Section 4. The systematic uncertainties are summarized in Section 5. The statistical methods and the results of the search are presented in Section 6. Conclusions are given in Section 7.

## 2 Photon Reconstruction, Event Selection and Sample Composition

### 2.1 Photon Reconstruction and Event Selection

The data used in this analysis were recorded using a diphoton trigger with a threshold on the transverse energy $E_{\mathrm{T}}$ on each photon of 20 GeV , seeded by a trigger that required two clusters in the electromagnetic calorimeter with $E_{\mathrm{T}}>12$ or 14 GeV , depending on the data-taking period. The trigger has an efficiency of approximately $99 \%$ for the signal after the final offline event selection. After applying data quality requirements on the recorded data sample, the total integrated luminosity of the data set used in this analysis amounts to $4.9 \mathrm{fb}^{-1}$.

Events are required to contain at least one primary vertex with at least three associated tracks, where the transverse momentum, $p_{\mathrm{T}}$, of each track is required to be larger than 0.4 GeV . Photons are reconstructed both in the converted and unconverted topologies. In both cases, photon candidates are seeded by energy clusters in the electromagnetic calorimeter with $E_{\mathrm{T}}>2.5 \mathrm{GeV}$. In the case of converted photon candidates, tracks reconstructed in the inner detector are matched to these calorimeter clusters. The photon energy is calibrated based on detailed Monte Carlo (MC) simulations, separately for converted and unconverted photons [8]. A correction, dependent on pseudorapidity and typically of the order of $\pm 1 \%$, is applied to the photon calibrated energy, as obtained from studies using $Z \rightarrow e e$ decays in data [9]. Photons are reconstructed in the fiducial region defined by the pseudorapidity ${ }^{1}|\eta|<2.37$, excluding the calorimeter barrel/endcap transition region, $1.37<|\eta|<1.52$.

The $E_{\mathrm{T}}$ of the leading (subleading) photon candidate must exceed 40 GeV ( 25 GeV ). MC simulation studies [8] have shown that this requirement leads to an optimal sensitivity in the mass region of interest. Both candidates are required to pass tight identification criteria based on shower shape variables and on the energy leakage into the hadronic calorimeter [10]. The tight photon identification efficiency ranges typically from $65 \%$ to $95 \%$ for $E_{\mathrm{T}}=25-80 \mathrm{GeV}$. These two photon candidates are required to be isolated by having at most 5 GeV energy deposited in the calorimeter in a cone of $\Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}=0.4$ around the candidate excluding the photon energy itself. The isolation variable is corrected for lateral shower leakage and ambient energy from pileup, as explained in Ref. [11]. The isolation cut efficiency for the diphoton candidate is $\approx 87 \%$ for the Higgs boson signal. If the reconstructed photon is a conversion, it is rejected if it has a track reconstructed in a region of the inner detector where the module traversed

[^66]in the innermost pixel layer is one of the $\approx 3.5 \%$ which are inactive, to reduce the contamination from misidentified electrons

The angle between the two selected photons is determined from the interaction vertex position and the photon impact points in the calorimeter. For converted photons with tracks having a precise measurement in the $z$ direction, the vertex position is estimated from the intercept of the line joining the reconstructed conversion position and the calorimeter impact point with the beam line. For all other photons, the vertex position is estimated from the shower position measurements in the first and second layers of the calorimeter which can be used to calculate the photon direction. Finally, the independent vertex position measurements from both photons are combined also taking into account the average beam spot position in $z$. For photons reconstructed in the endcap region, a correction is applied to the $z$ coordinate of the vertex position estimated from the photon in order to compensate for a difference between data and MC simulation. This correction is determined as a function of $\eta$ from electrons in $Z \rightarrow e e$ decays.

The diphoton invariant mass distribution ( $m_{\gamma \gamma}$ ) is shown in Figure 1 (top) for the 22489 events passing the selection in the mass region $100 \mathrm{GeV}<m_{\gamma \gamma}<160 \mathrm{GeV}$. The sum of the background-only fits in different categories described in Sections 3 and 4, as well as the signal expectation for a SM Higgs boson with mass equal to 120 GeV , are also shown. Details of the background and signal models are given in Section 4. Figure 1 (bottom) shows the residual of the data with respect to the sum of the backgroundonly fits as a function of $m_{\gamma \gamma}$.


Figure 1: Invariant mass distribution for the inclusive data sample, overlaid with the sum of the background-only fits in different categories described in Sections 3 and 4 and the signal expectation for a mass hypothesis of 120 GeV corresponding to the SM cross section. The figure below displays the residual of the data with respect to the background-only fit sum.

### 2.2 Sample Composition

The composition of the inclusive sample, after the selection described above, is studied using different data-driven techniques. The estimates obtained with these methods, however, are not used in the limit calculation described in Section 6.

The background to a potential Higgs boson signal is expected to be mainly composed of the diphoton processes $(\gamma \gamma)$ together with events where either of the photon candidates come from misidentified jets (fake photons), mainly through fragmentation into $\pi^{0}(\gamma j$ and $j j)$. A very small fraction of the background is due to misidentified electrons.

A double two-dimensional sideband method is used to extrapolate the jet backgrounds from control regions into the signal region by classifying the leading and subleading photon candidates into those passing or failing the isolation and tight identification cuts [7]. Events with diphotons from possible Higgs boson decays and misidentified Drell-Yan (DY) events (see discussion below), as well as prompt diphoton production events, are classified as $\gamma \gamma$ events. The estimation of each composition is performed in each bin of the $m_{\gamma \gamma}$ distribution. By construction, the sum of the components in each bin of the $m_{\gamma \gamma}$ distribution amounts exactly to the number of events in that bin. Systematic uncertainties arise mainly from variations of the control samples and a MC-based estimation of the diphoton event fraction in the regions dominated by jets.

The Drell-Yan background is studied separately by selecting $Z \rightarrow e e$ decays in data where either one or both electrons pass the photon selection. In this way an $e \rightarrow \gamma$ misidentification rate is obtained and the number of $Z \rightarrow e e$ events where both electrons are misidentified as photons is estimated.

The sample composition in bins of $m_{\gamma \gamma}$ is shown in Figure 2. The composition of the entire sample is summarized in Table 1. The diphoton purity is estimated to be $(71 \pm 5) \%$ in the full data sample, and consistent values are found in subsamples with different amounts of pileup. The event fractions of each component estimated with MC simulations are consistent with these data-driven results.

The sample composition is also studied with other two data-driven methods. The first one is a twodimensional fit method fitting simultaneously the isolation distributions of leading and subleading photon candidates with templates obtained from control samples [12]. The second method measures the rate of jets which are misidentified as photons in $W(\rightarrow e v)+\mathrm{jets}$ events and extrapolates the fake photon backgrounds into the signal region using a two-dimensional sideband technique. All methods give compatible results.

Table 1: Composition of the selected inclusive sample obtained from the measurement using the data as described in Section 2.2. The first uncertainty is statistical and the second systematic. Only the total uncertainty is quoted for the relative fractions.

| Composition | $\gamma \gamma$ | $\gamma j$ | $j j$ | Drell-Yan |
| :--- | :---: | :---: | :---: | :---: |
| Events | $16000 \pm 200 \pm 1100$ | $5230 \pm 130 \pm 880$ | $1130 \pm 50 \pm 600$ | $165 \pm 2 \pm 8$ |
| Relative fraction | $(71 \pm 5) \%$ | $(23 \pm 4) \%$ | $(5 \pm 3) \%$ | $(0.7 \pm 0.1) \%$ |

## 3 Event Categorization

In the previous analysis [7] events were divided according to the photon reconstruction topologies (converted, unconverted) and $\eta$ direction in five categories with different signal-to-background ratios and invariant mass resolutions:


Figure 2: Composition of the inclusive data sample as a function of $m_{\gamma \gamma}$, extracted from the double twodimensional sideband method after the inclusive event selection. The various components are stacked on top of each other. The error bars correspond to the statistical uncertainties on each component separately. The gray bands show the overall uncertainty on each component.

- Unconverted central: both photons are unconverted and located in the central part of the barrel calorimeter $(|\eta|<0.75)$. This is the category with the best invariant mass resolution;
- Unconverted rest: both photons are unconverted and at least one photon does not lie in the central part of the barrel calorimeter;
- Converted central: at least one photon is converted and both photons are found in the central part of the barrel calorimeter;
- Converted transition: at least one photon is converted and at least one photon is located near the transition between barrel and endcap calorimeter $(1.3<|\eta|<1.75)$. Given the larger amount of material in this region, the energy resolution, in particular for converted photons, can be significantly degraded;
- Converted rest: all other events with at least one converted photon.

With the increased data set corresponding to $4.9 \mathrm{fb}^{-1}$ it is possible to further split some of the categories to optimize the sensitivity to a potential Higgs boson signal. This analysis therefore introduces a new diphoton observable, $p_{\mathrm{Tt}}$, which is defined as the component of $\vec{p}_{\mathrm{T}}^{\gamma \gamma}$ transverse to the diphoton thrust axis [13, 14], as shown in Figure 3.


Figure 3: Sketch of the $p_{\mathrm{Tt}}$ definition.

The diphoton thrust axis, $\widehat{t}$, is defined as:

$$
\widehat{t}=\frac{\vec{p}_{\mathrm{T}}^{\gamma_{1}}-\vec{p}_{\mathrm{T}}^{\gamma_{2}}}{\left|\vec{p}_{\mathrm{T}}^{\gamma_{1}}-\vec{p}_{\mathrm{T}}^{\gamma_{2}}\right|}
$$

where the $\vec{p}_{T}^{\gamma_{1}}$ and $\vec{p}_{\mathrm{T}}^{\gamma_{2}}$ are the transverse momenta of the two selected photons. The transverse momentum of the diphoton system, $p_{\mathrm{T}}^{\gamma \gamma}$, is given by:

$$
\vec{p}_{\mathrm{T}}^{\gamma \gamma}=\vec{p}_{\mathrm{T}}^{\gamma_{1}}+\vec{p}_{\mathrm{T}}^{\gamma_{2}}
$$

The $p_{\mathrm{Tt}}$ is then calculated as follows:

$$
\begin{aligned}
\vec{p}_{\mathrm{Tt}} & =\vec{p}_{\mathrm{T}}^{\gamma \gamma}-\left(\vec{p}_{\mathrm{T}}^{\gamma \gamma} \cdot \widehat{t}\right) \cdot \widehat{t} \\
p_{\mathrm{Tt}} & =\left|\vec{p}_{\mathrm{T}}^{\gamma \gamma} \times \widehat{t}\right|
\end{aligned}
$$

Four of the aforementioned five categories are split into a low $p_{\mathrm{Tt}}$ category and a high $p_{\mathrm{Tt}}$ category, separated at $p_{\mathrm{Tt}}=40 \mathrm{GeV}$. The categorization based on the $p_{\mathrm{Tt}}$ variable leads to a better sensitivity for the Higgs boson signal than one based on $p_{\mathrm{T}}^{\gamma \gamma}$ due to the resolution of $p_{\mathrm{Tt}}$ being better than that of $p_{\mathrm{T}}^{\gamma \gamma}$. Moreover, the shape of the $m_{\gamma \gamma}$ distribution based on the $p_{\mathrm{Tt}}$ categorization can be better described with an exponential shape, which is not the case for the $p_{\mathrm{T}}^{\gamma \gamma}$ categorization. By introducing these $p_{\mathrm{Tt}}$ categories, the expected sensitivity of the analysis is improved by $5-10 \%$ depending on the hypothesized Higgs boson mass. The number of data events in each of the nine categories are shown in Table 2.

Table 2: The number of events found in $4.9 \mathrm{fb}^{-1}$ of data for the nine categories.

| Category | Conversion and $\eta$ | $p_{\mathrm{Tt}}$ cut | Number of data events |
| :---: | :--- | :---: | :---: |
| CP1 | Unconverted central | $p_{\mathrm{Tt}} \leq 40 \mathrm{GeV}$ | 1763 |
| CP2 | Unconverted central | $p_{\mathrm{Tt}}>40 \mathrm{GeV}$ | 235 |
| CP3 | Unconverted rest | $p_{\mathrm{Tt}} \leq 40 \mathrm{GeV}$ | 6234 |
| CP4 | Unconverted rest | $p_{\mathrm{Tt}}>40 \mathrm{GeV}$ | 1006 |
| CP5 | Converted central | $p_{\mathrm{Tt}} \leq 40 \mathrm{GeV}$ | 1318 |
| CP6 | Converted central | $p_{\mathrm{Tt}}>40 \mathrm{GeV}$ | 184 |
| CP7 | Converted rest | $p_{\mathrm{Tt}} \leq 40 \mathrm{GeV}$ | 7311 |
| CP8 | Converted rest | $p_{\mathrm{Tt}}>40 \mathrm{GeV}$ | 1072 |
| CP9 | Converted transition | No cut | 3366 |
| Total |  |  | 22489 |

## 4 Signal and Background Modelling

### 4.1 Signal Model

The Higgs boson signal is studied using MC samples which are then passed through a full detector simulation [15] using Geant 4 [16]. POWHEG [17] is used for gluon fusion and vector boson fusion (VBF) production, interfaced with PYTHIA [18] for showering and hadronization. PYTHIA is used to
generate the associated Higgs boson production modes ( $\mathrm{WH}, \mathrm{ZH}$ and ttH ). Pileup effects are simulated by overlaying each MC event with a variable number of MC inelastic proton-proton collisions [19], taking into account both in-time and out-of-time pileup and the LHC bunch train structure. The predicted signal is normalised using NNLO cross section predictions for the gluon fusion [20-23], VBF [24] and W/Z associated production [25]. The cross section of the teth process is known at NLO [26]. The branching ratio of a Higgs boson decaying to two photons is taken from Refs. [27, 28].

Signal samples are produced in 5 GeV steps of Higgs boson mass between 110 GeV and 150 GeV , and the following corrections are applied to these samples to match, as closely as possible, the conditions found in the data:

- The shower shape variables used in the photon identification are shifted to better resemble the corresponding distributions in the data [10]. The photon identification efficiency was cross-checked in data measurements using electrons in $Z \rightarrow e e$ and photons in $Z \rightarrow \ell \ell(\ell=e, \mu)$. Where simple shifts of the shower shape variables are insufficient to reproduce the data results, additional MC reweighing is used.
- The photon energy is smeared to account for small differences in resolution between data and simulation observed in studies of data $Z \rightarrow e e$ events [7];
- The MC samples are reweighted to reproduce the average number of interactions per bunch crossing observed in the data. The average number is approximately 6 until the end of August and then approximately 12 until the end of the proton-proton collision data-taking in 2011;
- The signal samples were produced with a longitudinal beam spot distribution corresponding to a Gaussian with width $\sigma_{z} \sim 7.5 \mathrm{~cm}$, which is larger than that observed in the data ( $\sigma_{z} \sim 6 \mathrm{~cm}$ ). The MC samples are therefore reweighted to correct for this difference;
- The MC signal yields are rescaled by the data-to-MC ratio for the isolation cut efficiency, as determined from $Z \rightarrow e e$ events. The shift evaluated from the isolation distribution of electrons between data and MC simulation is applied to the isolation variable of photons in the Higgs boson signal MC samples. This gives a $4.4 \%$ reduction in the expected signal yield;
- The MC samples for the gluon fusion process are reweighted to take into account the expected destructive interference between the $g g \rightarrow \gamma \gamma$ continuum background and the $g g \rightarrow H \rightarrow \gamma \gamma$ process [29]. The correction depends on the Higgs mass and the $\eta$ of the photons and is in the range 2-5\%;
- Events from the gluon fusion process are reweighted so that the distribution of the Higgs boson $p_{\mathrm{T}}$ matches that obtained from the HqT calculation [30].

The expected number of signal events for any given value of $m_{H}$ is obtained by a 3rd order polynomial fit to the signal yields extracted from the simulated samples. The number of expected signal events in each category is given in Table 3. The signal shapes as a function of $m_{\gamma \gamma}$ in each category are obtained from a simultaneous fit to the $m_{\gamma \gamma}$ distributions for all the generated Higgs boson mass points using the sum of a Crystal Ball (CB) function [31] and a wide but small amplitude Gaussian component describing the tails. The CB function is defined as:

$$
N \cdot \begin{cases}e^{-t^{2} / 2} & \text { if } t>-\alpha_{\mathrm{CB}}, \\ \left(\frac{n_{\mathrm{CB}}}{\alpha_{\mathrm{CB}}}\right)^{n_{\mathrm{CB}}} \cdot e^{-\alpha_{\mathrm{CB}}^{2} / 2} \cdot\left(\frac{n_{\mathrm{CB}}}{\alpha_{\mathrm{CB}}}-\alpha_{\mathrm{CB}}-t\right)^{-n_{\mathrm{CB}}} & \text { otherwise }\end{cases}
$$

where $t=\left(m_{\gamma \gamma}-m_{H}-\delta_{\mathrm{m}_{\mathrm{H}}}\right) / \sigma_{\mathrm{CB}}, N$ is a normalization parameter, $\delta_{\mathrm{m}_{\mathrm{H}}}$ is a category dependent offset, $\sigma_{\mathrm{CB}}$ represents the diphoton invariant mass resolution, and $n_{\mathrm{CB}}$ and $\alpha_{\mathrm{CB}}$ parametrize the non-Gaussian

Table 3: Expected Higgs boson signal yields after full event selection in $4.9 \mathrm{fb}^{-1}$ integrated over a mass range of $100-160 \mathrm{GeV}$ for various values of $m_{H}$ in each category and the sum.

| $m_{H}[\mathrm{GeV}]$ | 110 | 115 | 120 | 125 | 130 | 135 | 140 | 145 | 150 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{CP} 1:$ Unconverted central, low $p_{\mathrm{Tt}}$ | 8.9 | 8.9 | 8.7 | 8.2 | 7.5 | 6.7 | 5.7 | 4.6 | 3.5 |
| CP : Unconverted central, high $p_{\mathrm{Tt}}$ | 2.5 | 2.6 | 2.6 | 2.5 | 2.3 | 2.1 | 1.8 | 1.5 | 1.2 |
| CP : Unconverted rest, low $p_{\mathrm{Tt}}$ | 16.3 | 16.7 | 16.6 | 16.0 | 15.0 | 13.6 | 11.9 | 9.8 | 7.4 |
| $\mathrm{CP} 4:$ Unconverted rest, high $p_{\mathrm{Tt}}$ | 4.4 | 4.6 | 4.6 | 4.5 | 4.3 | 4.0 | 3.5 | 2.9 | 2.2 |
| CP : Converted central, low $p_{\mathrm{Tt}}$ | 5.9 | 5.9 | 5.8 | 5.5 | 5.1 | 4.6 | 4.0 | 3.3 | 2.4 |
| CP : Converted central, high $p_{\mathrm{Tt}}$ | 1.6 | 1.7 | 1.6 | 1.6 | 1.6 | 1.4 | 1.3 | 1.1 | 0.8 |
| CP 7 : Converted rest, low $p_{\mathrm{Tt}}$ | 17.5 | 18.1 | 17.9 | 17.1 | 15.8 | 14.1 | 12.0 | 9.7 | 7.2 |
| $\mathrm{CP}:$ Converted rest, high $p_{\mathrm{Tt}}$ | 4.6 | 4.7 | 4.7 | 4.6 | 4.4 | 4.1 | 3.6 | 2.9 | 2.2 |
| $\mathrm{CP9}:$ Converted transition | 8.2 | 8.4 | 8.4 | 8.1 | 7.6 | 6.9 | 6.0 | 4.9 | 3.7 |
| Total | 69.9 | 71.5 | 70.9 | 68.3 | 63.7 | 57.5 | 49.8 | 40.8 | 30.6 |

tail. The variables $\delta_{\mathrm{m}_{\mathrm{H}}}, \sigma_{\mathrm{CB}}$ and $\alpha_{\mathrm{CB}}$ of the CB function depend linearly on the Higgs boson mass. The mean and $\sigma$ of the additional Gaussian function are constrained to the value of $m_{H}+\delta_{\mathrm{m}_{\mathrm{H}}}$ and $\kappa \cdot \sigma_{\mathrm{CB}}$. The variables $\delta_{\mathrm{m}_{\mathrm{H}}}, \sigma_{\mathrm{CB}}, \alpha_{\mathrm{CB}}$ and $\kappa$ and a fraction of the component of the CB function are determined with the simultaneous fit fixing $n_{\mathrm{CB}}$ to be 10 . The core component of the mass resolution, $\sigma_{\mathrm{CB}}$, ranges from 1.4 GeV in the "Unconverted Central" categories to 2.3 GeV in the "Converted Transition" category over the full mass range that is studied. The effect of the pileup on the mass resolution is negligible.

The result of the simultaneous fit for events selected with the inclusive analysis (i.e. without categorization) for a mass hypothesis of 120 GeV is displayed in Figure 4. Table 4 summarizes the mass resolution, $\sigma_{\mathrm{CB}}$ and full width half-maximum ( FWHM ), the expected number of signal events, the estimated number of background events in each category as determined from the data (Section 4.2), and their ratio in the mass window of $\pm 1.4 \sigma_{\mathrm{CB}}$, for a Higgs signal of $m_{H}=120 \mathrm{GeV}$.

### 4.2 Background Model

The background is estimated from the data by fitting the diphoton mass spectrum in the whole range of $100-160 \mathrm{GeV}$ with a single exponential function. Such a function was found to describe all the categories very well, as obtained from studies using large samples of diphoton events produced by the RESBOS [32] and DIPHOX [33] MC generators. Figures 5 and 6 show the invariant mass spectra reconstructed in data and the results of the unbinned maximum likelihood fit under the background-only hypothesis for the nine categories.

The systematic uncertainty on the background modelling is assigned by estimating, for each category, the potential difference between the true background shape and the single exponential function which could fake a signal-like signature. This is obtained from MC by calculating the difference between the mass distributions of the events generated with RESBOS and DIPHOX and the result of the exponential fit to these distributions. The maximum difference integrated over a window of 4 GeV normalised to the total event count in each category is assigned as uncertainty (Table 5). Other functional forms, including $2^{\text {nd }}$ order Bernstein polynomials and double exponential functions, were fitted to the data and compared to the exponential fit. The uncertainties arising from these comparisons were found to be of similar size to the MC-based estimate.


Figure 4: Reconstructed inclusive invariant mass distribution for a simulated signal of $m_{H}=120 \mathrm{GeV}$. The result of the simultaneous fit to all Higgs boson mass points is superimposed. The core component of the mass resolution, $\sigma_{\mathrm{CB}}$, is 1.7 GeV and the FWHM of the distribution is 4.0 GeV .

Table 4: The mass resolution of Higgs signal events ( $\sigma_{\mathrm{CB}}$ and FWHM), the expected number of signal events ( $N_{\mathrm{sig}}$ ), the estimated number of background events ( $N_{\mathrm{BG}}$ ) from data, and their ratio $\left(N_{\text {sig }} / N_{\mathrm{BG}}\right)$ in the mass window of $\pm 1.4 \sigma_{\mathrm{CB}}$ for $m_{H}=120 \mathrm{GeV}$ corresponding to an integrated luminosity of $4.9 \mathrm{fb}^{-1}$.

| Category | $\sigma_{\mathrm{CB}}[\mathrm{GeV}]$ | FWHM [GeV] | $N_{\text {sig }}$ | $N_{\text {BG }}$ | $N_{\text {sig }} / N_{\text {BG }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| CP 1 : Unconverted central, low $p_{\mathrm{Tt}}$ | 1.4 | 3.4 | 7.3 | 142 | 0.051 |
| CP 2 : Unconverted central, high $p_{\mathrm{Tt}}$ | 1.4 | 3.3 | 2.2 | 18 | 0.117 |
| CP3: Unconverted rest, low $p_{\mathrm{Tt}}$ | 1.7 | 4.1 | 13.5 | 589 | 0.023 |
| CP4: Unconverted rest, high $p_{\text {Tt }}$ | 1.6 | 3.9 | 3.8 | 87 | 0.043 |
| CP5: Converted central, low $p_{\mathrm{Tt}}$ | 1.7 | 3.9 | 4.7 | 125 | 0.038 |
| CP6: Converted central, high $p_{\text {Tt }}$ | 1.6 | 3.7 | 1.4 | 16 | 0.085 |
| CP7: Converted rest, low $p_{\text {Tt }}$ | 2.0 | 4.7 | 14.0 | 805 | 0.017 |
| CP8: Converted rest, high $p_{\mathrm{Tt}}$ | 1.9 | 4.5 | 3.7 | 110 | 0.034 |
| CP9: Converted transition | 2.3 | 5.8 | 5.9 | 429 | 0.014 |

Table 5: Systematic uncertainty (the number of events for data of $4.9 \mathrm{fb}^{-1}$ ) on the background modelling in different categories.

| Category | CP1 | CP2 | CP3 | CP4 | CP5 | CP6 | CP7 | CP8 | CP9 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Events | $\pm 4.3$ | $\pm 0.2$ | $\pm 3.7$ | $\pm 0.5$ | $\pm 3.2$ | $\pm 0.1$ | $\pm 5.6$ | $\pm 0.6$ | $\pm 2.3$ |

## 5 Systematic Uncertainties

Systematic uncertainties affecting the extraction of a possible signal from the diphoton invariant mass distribution related to the modelling of the signal itself can be classified into three types: uncertainties


Figure 5: Diphoton invariant mass distributions for the data (points with error bars) for the four "unconverted" categories (CP1-CP4). For each plot the line shows the result of the exponential fit.
on the predicted yield, uncertainties on the signal invariant mass resolution and uncertainties on event migration between categories.

The uncertainties on the predicted signal yield are the following:

- $\mathrm{A} \pm 11 \%$ uncertainty from the photon reconstruction and identification. This is estimated by comparing the MC-based efficiencies with those extrapolated from measurement of electrons from $W / Z$-boson decays, and with the direct measurements of photons in $Z \rightarrow \ell \ell \gamma(\ell=e, \mu)$ decays which only cover the $E_{\mathrm{T}}$ range $25-60 \mathrm{GeV}$. The impact of possible additional material in front of the calorimeter, as estimated with MC simulations, is also included;
- A $\pm 4 \%$ uncertainty from the effect of the pileup on the photon reconstruction and identification efficiency. This is estimated by looking at the variation of the tight photon identification efficiency as a function of the average number of interactions per bunch crossing;
- The effect of the photon energy scale uncertainty $(\approx 0.5 \%)$ was found be to small $(0.3 \%)$, and is therefore neglected;
- A $\pm 5 \%$ uncertainty on the isolation cut efficiency. This is estimated from the difference between the isolation cut efficiency in data and MC simulation using $Z \rightarrow e e$ events;
- $\mathrm{A} \pm 1 \%$ uncertainty on the trigger efficiency. This comes from the uncertainty in the measurement of the trigger efficiency for diphoton candidates using control triggers, and from possible differ-


Figure 6: Diphoton invariant mass distributions for the data (points with error bars) for the five "converted" categories (CP5-CP9). For each plot the line shows the result of the exponential fit.
ences, evaluated with MC samples, between the trigger efficiency for photons from Higgs boson decays and for photons from all diphoton candidates;

- $\mathrm{A}+15 \% /-11 \%$ uncertainty on the signal cross section [27]. This is evaluated by varying the renormalization and factorization scales and using different parton distributions (PDF) [34] in the gluon fusion process, which has the largest uncertainty compared to other processes and dominates in all the categories ( $95 \%$ for low $p_{\mathrm{Tt}}$ and $80 \%$ for low $p_{\mathrm{Tt}}$ ). The same uncertainty is applied to signal samples produced with other processes;
- $\mathrm{A} \pm 1 \%$ uncertainty on the signal acceptance from the modelling of the Higgs boson $p_{\mathrm{T}}$, which is estimated by comparing the predictions of the HqT [30] and RESBOS [35] programs;
- A $\pm 3.9 \%$ overall uncertainty on the total integrated luminosity in the full 2011 data set, as extrapolated from Ref. [36].

The uncertainties on the mass resolution arise from the following:

- A $\pm 12 \%$ uncertainty from the calorimeter energy resolution. This results from the uncertainty on the sampling term, which is estimated to be $\pm 10 \%$, and from the uncertainty on the constant term, which is estimated to be $\left(1.2_{-0.6}^{+0.5}\right) \%$ for the barrel and $(1.8 \pm 0.6) \%$ for the endcap calorimeter using $Z \rightarrow e e$ events [9];
- A $\pm 6 \%$ uncertainty arising from the extrapolation of the electron energy calibration to that for photons. This extrapolation, obtained from MC studies, is affected by the imperfect knowledge of the material in front of the active part of the calorimeter. The effect of this imperfect knowledge on the mass resolution is evaluated using simulations with a different amount of material in front of the calorimeter.
- A $\pm 3 \%$ uncertainty from the effect of the pileup on the energy resolution. Pileup fluctuations contributing to the cluster energy measurement were checked using reconstructed clusters in randomlytriggered bunch crossings, selected in proportion to the instantaneous luminosity in the data [7];
- $\mathrm{A} \pm 1 \%$ uncertainty from the photon angle measurement on the mass resolution. This was studied in $Z \rightarrow e e$ events comparing track-based with calorimeter-based direction measurements [7].

The uncertainties on the event migration between categories arise from the following:

- $\mathrm{A} \pm 8 \%$ migration of events from the high $p_{\mathrm{Tt}}$ categories to the low $p_{\mathrm{Tt}}$ categories. This is estimated from gluon fusion Higgs boson signal MC events by varying the renormalization, factorization and resummation scales and PDF choices for the modelling of the $p_{\mathrm{T}}^{\gamma \gamma}$ spectrum in the Hq T program. The same uncertainty is applied to signal samples produced with other processes. The effect of photon energy scale uncertainty on this migration is small $(0.5 \%)$ and is neglected;
- $\mathrm{A} \pm 4.5 \%$ migration of events from the unconverted categories to the converted categories. The impact of pileup and additional material in front of the calorimeter is estimated from MC samples with different pileup and material configurations.

The systematic uncertainties on the expected signal are summarized in Table 6. Systematic uncertainties on the event yield and the mass resolution are taken as fully correlated between different categories, while those on the event migration are anti-correlated between the high and low $p_{\mathrm{Tt}}$ categories and between the unconverted and converted categories. Systematic uncertainties on the background modelling yield between $\pm 0.1$ and $\pm 5.6$ events depending on the category (Table 5). These uncertainties are treated as uncorrelated between categories except for those that share the same $\eta$ and $p_{\mathrm{Tt}}$ classification but different conversion status.

## 6 Results

The statistical interpretation of the data follows the procedure described in Ref. [5] which adopts a modified frequentist approach $\left(C L_{S}\right)$ [37] for setting the limit and a frequentist approach to calculate the $p_{0}$-value. The combined likelihood function is constructed from the likelihood functions of the nine categories, and the systematic uncertainties are incorporated by introducing 31 nuisance parameters with

Table 6: Summary of systematic uncertainties on the expected signal.

| Type and source | Uncertainty |
| :--- | :---: |
| Event yield |  |
| Photon reconstruction and identification | $\pm 11 \%$ |
| Effect of pileup on photon identification | $\pm 4 \%$ |
| Isolation cut efficiency | $\pm 5 \%$ |
| Trigger efficiency | $\pm 1 \%$ |
| Higgs boson cross section | $+15 \% /-11 \%$ |
| Higgs boson $p_{\mathrm{T}}$ modeling | $\pm 1 \%$ |
| Luminosity | $\pm 3.9 \%$ |
| Mass resolution |  |
| Calorimeter energy resolution | $\pm 12 \%$ |
| Photon energy calibration | $\pm 6 \%$ |
| Effect of pileup on energy resolution | $\pm 3 \%$ |
| Photon angular resolution | $\pm 1 \%$ |
| Migration |  |

Gaussian constraints. Asymptotic formulae [38] were used to derive the limit and $p_{0}$-values, and pseudoexperiments were generated to confirm the validity of this procedure.

The $p_{0}$-value, used to quantify the probability of seeing an excess at least as large as this in the background-only hypothesis, is evaluated for Higgs boson mass hypotheses between 110 GeV and 150 GeV in steps of 1 GeV . The expected and observed $p_{0}$-values are shown in Figure 7. The expected $p_{0}$-value is evaluated assuming a SM Higgs boson signal plus background for a given hypothesized Higgs boson mass. The minimal observed $p_{0}$-value is $0.27 \%$ and is found for a mass hypothesis of $m_{H}=126 \mathrm{GeV}$. This $p_{0}$-value corresponds to 2.8 standard deviations. The probability of such an excess appearing anywhere in the mass range investigated due to a background fluctuation, accounting for the look-elsewhere effect, is estimated to be approximately $7 \%$ and it reduces the observed significance to 1.5 standard deviations. This was determined using the prescription described in Ref. [39]. As cross checks, the observed $p_{0}$-values were reevaluated using alternate background models, including the $2^{\text {nd }}$ order Bernstein polynomials. Also, the uncertainties on the background modelling due to the use of a single exponential (Table 5) were set to zero or doubled. Furthermore, a photon energy scale uncertainty of $\approx 0.5 \%$ was introduced into the likelihood fits. All of these checks gave observed $p_{0}$-values which are similar to the quoted result. The largest change in the observed significance at $m_{H}=126 \mathrm{GeV}$ was 0.16 standard deviations.

The $95 \%$ confidence level (CL) limits on the ratio of the inclusive production cross section of a SMlike Higgs boson relative to the SM cross section are also derived as shown in Figure 8. The expected limits vary between 1.6 and 1.8 times the predicted SM cross section in the mass range $115-130 \mathrm{GeV}$, and between 1.6 and 2.9 times the SM cross section over the full mass range that is studied. The observed limits are set between 0.9 and 4.0 times the SM cross section over the full mass range. A SM Higgs boson in the mass ranges $114-115 \mathrm{GeV}$ and $135-136 \mathrm{GeV}$ is excluded. The numerical values of the limits and $p_{0}$-values in steps of 1 GeV are listed in Table 7.


Figure 7: The observed and expected $p_{0}$-value as a function of the hypothesized Higgs boson mass without taking the look-elsewhere effect into account. The dotted-dashed lines indicate the corresponding significance.

## 7 Conclusions

A search for the SM Higgs boson in the diphoton decay channel has been performed using data corresponding to an integrated luminosity of $4.9 \mathrm{fb}^{-1}$ recorded by the ATLAS experiment in 2011. Over the diphoton mass range $110-150 \mathrm{GeV}$ the maximum deviation from the background-only expectation is observed at 126 GeV with a local significance of 2.8 standard deviations. Taking the look-elsewhere effect into account, the significance is 1.5 standard deviations. The expected cross section exclusion at $95 \%$ confidence level varies between 1.6 and 1.8 times the SM cross section in the mass range $115-130 \mathrm{GeV}$, and between 1.6 and 2.9 over the full mass range that is studied. The observed exclusions are set between 0.9 and 4.0 times the SM cross section over the full mass range. A SM Higgs boson is excluded at $95 \%$ CL in the mass ranges of $114-115 \mathrm{GeV}$ and $135-136 \mathrm{GeV}$.


Figure 8: The observed and expected $95 \%$ confidence level limits, normalised to the SM Higgs boson cross sections, as a function of the hypothesized Higgs boson mass.

Table 7: The expected and observed limits, normalised to the Higgs boson cross section as predicted by the SM, and the observed and expected (for a SM Higgs boson) $p_{0}$-values.

| $m_{H}[\mathrm{GeV}]$ | Expected limit | Observed limit | Expected $p_{0}$ | Observed $p_{0}$ |
| :---: | :---: | :---: | :---: | :---: |
| 110 | 2.01 | 1.94 | 0.15 | 0.50 |
| 111 | 1.95 | 1.67 | 0.15 | 0.50 |
| 112 | 1.90 | 1.32 | 0.14 | 0.50 |
| 113 | 1.85 | 1.01 | 0.13 | 0.50 |
| 114 | 1.82 | 0.86 | 0.13 | 0.50 |
| 115 | 1.78 | 0.93 | 0.12 | 0.50 |
| 116 | 1.74 | 1.28 | 0.12 | 0.50 |
| 117 | 1.72 | 1.83 | 0.11 | 0.46 |
| 118 | 1.70 | 2.12 | 0.11 | 0.29 |
| 119 | 1.67 | 1.85 | 0.10 | 0.42 |
| 120 | 1.66 | 1.41 | 0.10 | 0.50 |
| 121 | 1.65 | 1.15 | 0.097 | 0.50 |
| 122 | 1.64 | 1.23 | 0.094 | 0.50 |
| 123 | 1.63 | 1.73 | 0.093 | 0.48 |
| 124 | 1.63 | 2.62 | 0.092 | 0.11 |
| 125 | 1.61 | 3.55 | 0.092 | 0.013 |
| 126 | 1.61 | 4.04 | 0.089 | 0.0027 |
| 127 | 1.63 | 3.82 | 0.089 | 0.0055 |
| 128 | 1.63 | 3.06 | 0.089 | 0.053 |
| 129 | 1.64 | 2.19 | 0.091 | 0.27 |
| 130 | 1.65 | 1.65 | 0.093 | 0.50 |
| 131 | 1.66 | 1.43 | 0.095 | 0.50 |
| 132 | 1.67 | 1.34 | 0.096 | 0.50 |
| 133 | 1.69 | 1.28 | 0.096 | 0.50 |
| 134 | 1.71 | 1.14 | 0.10 | 0.50 |
| 135 | 1.73 | 0.98 | 0.10 | 0.50 |
| 136 | 1.77 | 0.95 | 0.10 | 0.50 |
| 137 | 1.79 | 1.21 | 0.11 | 0.50 |
| 138 | 1.83 | 1.68 | 0.11 | 0.50 |
| 139 | 1.88 | 1.96 | 0.11 | 0.41 |
| 140 | 1.91 | 1.76 | 0.12 | 0.50 |
| 141 | 1.97 | 1.46 | 0.12 | 0.50 |
| 142 | 2.03 | 1.46 | 0.13 | 0.50 |
| 143 | 2.09 | 1.87 | 0.14 | 0.50 |
| 144 | 2.16 | 2.47 | 0.15 | 0.33 |
| 145 | 2.25 | 2.88 | 0.16 | 0.24 |
| 146 | 2.34 | 2.85 | 0.16 | 0.31 |
| 147 | 2.44 | 2.54 | 0.17 | 0.49 |
| 148 | 2.56 | 2.25 | 0.18 | 0.50 |
| 149 | 2.70 | 2.02 | 0.19 | 0.50 |
| 150 | 2.87 | 1.92 | 0.20 | 0.50 |

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## Appendix: Auxiliary public plots



Figure 9: The reconstructed diphoton mass in simulated $H \rightarrow \gamma \gamma$ events using the fit with the sum of a Crystal Ball function plus a Gaussian for the inclusive event selection. In the left plot, the method explained in Section 2.1 ("Calo/Conv pointing") is used to determine the vertex position. Four different results are shown corresponding to four different pile-up conditions. The number of average interactions per bunch crossing is denoted by $\mu$. On the right, the fit results using the vertex determined with "Calo/Conv pointing" method is compared to two other methods to deduce the angle between the photons. The truth vertex gives the best possible result by using MC truth information to deduce the correct primary vertex. In the $\Sigma p_{T}^{2}$ method the primary vertex is chosen as the one with the largest sum of the $p_{T}^{2}$ of the tracks associated to it. The improvement of the mass resolution by using the "Calo/Conv pointing" method instead of the $\Sigma p_{T}^{2}$ method amounts to $5-20 \%$, depending on the pile-up conditions.


Figure 10: Background components in the inclusive analysis extracted by the double two-dimensional sideband method for two data taking periods. The first period taken with LHC beam optics parameter $\beta^{*}=1.5 \mathrm{~m}$ corresponds to an integrated luminosity of $2.1 \mathrm{fb}^{-1}$ and on average 6 interactions per bunch crossing. The later period taken with $\beta^{*}=1.0 \mathrm{~m}$ corresponds to $2.8 \mathrm{fb}^{-1}$ and 12 interactions per bunch crossing on average. The statistical uncertainty is negligible small comparing to the systematic uncertainty.


Figure 11: Comparison of the number of background events for each component predicted using theory and MC simulation to the results of the data-driven data decomposition using the double two-dimensional sideband method. This is an update of the results in Ref. [1] using the full 2011 data sample.
[1] The ATLAS Collaboration, Search for the Higgs boson in the Diphoton Channel with the ATLAS Detector using $209 \mathrm{pb}^{-1}$ of 7 TeV Data taken in 2011, ATLAS-CONF-2011-085 (2011).


Figure 12: The observed and expected local $p_{0}$-value as a function of $m_{H}$ for three different background models without taking the look-elsewhere effect into account. The black solid line is the result described in detail in this note, using single exponential functions in all categories. In the Hybrid model the high $p_{\mathrm{Tt}}$ categories are fitted with the $2^{\text {nd }}$ order Bernstein polynomials, the other categories with the single exponential. In the model Bernstein all categories are fitted with the Bernstein function. The $p_{0}$-values near the minima at 126 GeV are very similar in all cases: $p_{0}=0.38 \%$ using the Hybrid model, and $p_{0}=0.25 \%$ using the Bernestein function.


Figure 13: Event display of a candidate diphoton event where both photon candidates are unconverted. The event number is 86694500 and it was recorded during run 191426. The leading photon has $E_{\mathrm{T}}=64.2 \mathrm{GeV}$ and $\eta=-0.34$. The subleading photon has $E_{\mathrm{T}}=61.4 \mathrm{GeV}$ and $\eta=-0.61$. The measured diphoton mass is 126.6 GeV . The $p_{\mathrm{T}}$ and $p_{\mathrm{Tt}}$ of the diphoton are 6.1 GeV and 5.4 GeV , respectively. Only reconstructed tracks with $p_{\mathrm{T}}>1 \mathrm{GeV}$, hits in the pixel and SCT layers and TRT hits with a high threshold are shown.


Figure 14: Event display of a candidate diphoton event where the leading (subleading) photon candidate is unconverted (converted). The event number is 19448322 and it was recorded during run 191190. The leading photon has $E_{\mathrm{T}}=66.8 \mathrm{GeV}$ and $\eta=-0.27$. The subleading photon has $E_{\mathrm{T}}=56.9 \mathrm{GeV}$ and $\eta=-$ 0.67. The measured diphoton mass is 125.8 GeV . The $p_{\mathrm{T}}$ and $p_{\mathrm{Tt}}$ of the diphoton are 10.4 GeV and 3.1 GeV , respectively. The conversion radius of the subleading photon is measured to be 8.1 cm . Only reconstructed tracks with $p_{\mathrm{T}}>1 \mathrm{GeV}$, hits in the pixel and SCT layers and TRT hits with a high threshold are shown.


Figure 15: Close-up view in the transverse plane of the converted photon candidate shown in Figure 14 (run number $=191190$, event number $=19448322$ ). Only reconstructed tracks with $p_{\mathrm{T}}>2 \mathrm{GeV}$ and $|\eta|<1.4$ are shown, and only the hits in the pixel, SCT and TRT layers with $-1<|\eta|<0$ are shown. Starting from the primary vertex (shown as a large magenta dot on the left), the photon conversion vertex (brown dot) can be seen at a radius of 8.1 cm , followed by the pixel hits (magenta dots), SCT clusters (green segments) and TRT hits (blue dots for normal $\mathrm{d} E / \mathrm{d} x$ hits and red dots for hits above the high threshold required for transition radiation). The electron track (blue line) has $p_{\mathrm{T}}=56.1 \mathrm{GeV}$ and matches well with the electromagnetic cluster (shown in yellow at the outer radius). The positron track has $p_{\mathrm{T}}=4.0 \mathrm{GeV}$ and a fraction of its energy actually lies outside the main cluster.


Figure 16: Close-up view in the transverse plane of the longitudinal shower profile in the barrel electromagnetic calorimeter of the converted photon candidate shown in Figure 14 (run number $=191190$, event number $=19448322$ ). The layers of the EM calorimeter are shown as green boxes with sizes representing their real dimensions and with heights proportional to the energy deposited (normalised differently for each layer for viewing purposes). The two electrons from the photon conversions encounter first the presampler layer (which provides an estimate of the energy lost by bremsstrahlung in front of the active calorimeter), then the strip layer, which is fine-grained in $\eta$ and provides good $\gamma / \pi^{0}$ rejection, and finally the second layer where most of the energy is deposited. The conversion is quite asymmetric and the showers initiated by the two electrons appear in different strip-layer modules (in $\phi$ ) but line up very well with each other in $\eta$, as expected for such an electron pair.

## ATLAS NOTE

ATLAS-CONF-2011-162

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# Search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ with $4.8 \mathbf{f b}^{-1}$ of pp collisions at $\sqrt{s}=7 \mathrm{TeV}$ 

The ATLAS collaboration


#### Abstract

A search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z^{(*)} \rightarrow$ $\ell^{+} \ell^{-} \ell^{\prime}+\ell^{\prime}-$, where $\ell, \ell^{\prime}=e, \mu$, is presented. Proton-proton collision data at $\sqrt{s}=7 \mathrm{TeV}$ recorded with the ATLAS detector and corresponding to an average integrated luminosity of $4.8 \mathrm{fb}^{-1}$ are compared to the Standard Model background expectations. Upper limits on the production cross section of a Standard Model Higgs boson with a mass between 110 GeV and 600 GeV are derived. The Standard Model Higgs boson is excluded at $95 \%$ confidence level in the mass ranges $135 \mathrm{GeV}-156 \mathrm{GeV}, 181 \mathrm{GeV}-234 \mathrm{GeV}$ and $255 \mathrm{GeV}-415 \mathrm{GeV}$. The largest deviations from the background expectation are observed for $m_{H}=125 \mathrm{GeV}$ with a $p_{0}$-value of $1.8 \%, m_{H}=244 \mathrm{GeV}$ with a $p_{0}$-value of $1.1 \%$ and $m_{H}=500 \mathrm{GeV}$ with a $p_{0}$-value of $1.4 \%$. Once the look-elsewhere effect is considered, none of these excesses is significant by itself.


## 1 Introduction

The search for the Standard Model (SM) Higgs boson [1-3] is a major goal of the Large Hadron Collider (LHC) programme. Direct searches at the CERN LEP $e^{+} e^{-}$collider excluded at $95 \%$ confidence level (CL) the production of a SM Higgs with $m_{H}<114.4 \mathrm{GeV}$ [4]. The searches at the Fermilab Tevatron $p \bar{p}$ collider have excluded at $95 \%$ CL the region $156 \mathrm{GeV}<m_{H}<177 \mathrm{GeV}$ [5]. At the LHC, the latest results of the ATLAS SM Higgs searches [6] based on data collected during the early part of the 2011 LHC run exclude the Higgs boson mass ( $m_{H}$ ) ranges $146-230 \mathrm{GeV}, 256-282 \mathrm{GeV}$ and $296-459 \mathrm{GeV}$ at $95 \%$ CL, while for CMS the corresponding excluded ranges are $145-216 \mathrm{GeV}, 226-288 \mathrm{GeV}$ and $310-400 \mathrm{GeV}$ [7]. A preliminary combination of $1.0-2.3 \mathrm{fb}^{-1}$ of LHC data per experiment exclude the SM Higgs in the region $141 \mathrm{GeV}<m_{H}<476 \mathrm{GeV}$ at $95 \%$ CL [8].

In ATLAS several final states are used to search for the SM Higgs boson [9-17]. The search for the SM Higgs through the decay $H \rightarrow \mathrm{ZZ}^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{\prime}+\ell^{\prime-}$, where $\ell, \ell^{\prime}=e, \mu$ provides good sensitivity in a wide mass range. The results of the previous search in this channel, with $2.1 \mathrm{fb}^{-1}$ [10], showed exclusion in three mass regions between 191 GeV and 224 GeV . This note presents an update of the ATLAS search for a SM Higgs boson in this channel for the mass range from 110 GeV to $600 \mathrm{GeV}^{1}$. Three distinct final states, $\mu \mu \mu \mu(4 \mu), e e \mu \mu(2 e 2 \mu)$, and eeee ( $4 e$ ), are selected. The largest background to this search comes from continuum $Z Z^{(*)}$ production. For $m_{H}<180 \mathrm{GeV}$, contributions from $Z+$ jets and $t \bar{t}$ processes, where the additional charged leptons arise either from decays of hadrons with heavy ( $b$ and $c$-quark) flavour content or from light-flavour-jets misidentified as leptons, are important. The $p p$ collision data were recorded with the ATLAS detector at the LHC at $\sqrt{s}=7 \mathrm{TeV}$ and correspond to an average integrated luminosity of $4.8 \mathrm{fb}^{-1}$ [18], more than twice that of Ref. [10]. With respect to Ref. [10] the electron identification has been refined to improve efficiency. The electron tracks have been refitted using the Gaussian Sum Filter [19,20] which corrects for energy losses due to bremsstrahlung, offering more accurate track parameter measurements. Moreover, the muon momentum resolution has improved due to improved alignment of the inner detector and muon spectrometer.

## 2 The ATLAS Detector

The ATLAS detector [21] is a multi-purpose particle physics apparatus with forward-backward symmetric cylindrical geometry ${ }^{2}$. The inner tracking detector (ID) consists of a silicon pixel detector, a silicon microstrip detector, and a transition radiation tracker. The ID is surrounded by a thin superconducting solenoid providing a 2 T magnetic field. A high-granularity lead-liquid argon (LAr) sampling calorimeter measures the energy and the position of electromagnetic showers. An iron-scintillator tile calorimeter provides hadronic coverage in the central rapidity range. The end-cap and forward rapidity regions are instrumented with LAr calorimetry for both electromagnetic and hadronic measurements. The muon spectrometer (MS) surrounds the calorimeters and consists of three large superconducting toroids, each with eight coils, a system of precision tracking chambers, and detectors for triggering. A three-level trigger system selects events to be recorded for offline analysis.

[^67]
## 3 Data and Simulation Samples

The accumulated data are subjected to quality requirements ensuring that the relevant detector components were operating normally. The resulting average integrated luminosity of $4.8 \mathrm{fb}^{-1}$ corresponds to $4.81 \mathrm{fb}^{-1}, 4.81 \mathrm{fb}^{-1}$ and $4.91 \mathrm{fb}^{-1}$ for the $4 \mu, 2 e 2 \mu$ and $4 e$ final states, respectively.

The $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ signal is modelled using the POWHEG Monte Carlo (MC) event generator [22, 23], which calculates separately the gluon and vector-boson fusion production mechanisms with matrix elements up to next-to-leading order (NLO). The Higgs boson transverse momentum, $p_{\mathrm{T}}$, spectrum in the gluon fusion process is reweighted to the calculation of Ref. [24], providing QCD corrections up to next-to-leading order and QCD soft-gluon resummations up to next-to-next-to-leading log (NNLL). POWHEG is interfaced to PYTHIA [25] for showering and hadronization, which in turn is interfaced to PHOTOS [26] for QED radiative corrections in the final state and to TAUOLA [27, 28] for the simulation of $\tau$ decays. For the Higgs boson associated production with a $W$ or a $Z$ boson, PYtHIA is used.

The cross sections for Higgs boson production, the corresponding branching fractions, as well as their uncertainties [29], are derived to next-to-next-to-leading order (NNLO) in QCD for the gluon fusion [30-35], vector-boson fusion [36] and the associated production with a $W$ or $Z$ boson [37] processes. In addition, QCD soft-gluon resummations up to NNLL are available for the gluon fusion process [38], while the NLO electroweak (EW) corrections are applied to the gluon fusion [39, 40], the vector-boson fusion [41, 42] and the associated production with a $W$ or $Z$ boson [43] processes. These cross section calculations do not take into account the width of the Higgs boson, which is implemented through a Breit-Wigner line shape applied at the event generator level. Recent studies [44-46] have indicated that effects related to off-shell Higgs boson production and interference with other SM processes may become sizeable at the highest masses $\left(m_{H}>400 \mathrm{GeV}\right)$ considered in this search. In the absence of a full calculation, a conservative estimate of the possible size of such effects was included as a signal normalization systematic uncertainty following a parameterization as a function of $m_{H}: 150 \% \times\left(m_{H}[\mathrm{TeV}]\right)^{3}$, for $m_{H} \geq 300 \mathrm{GeV}$ [47]. The Higgs boson decay branching ratio to the four-lepton final state is predicted by PROPHECY4F [48,49], which includes the complete NLO QCD+EW corrections, interference effects between identical final state fermions and leading two-loop heavy Higgs boson corrections to the fourfermion width. Table 1 gives the production cross sections and branching ratios for $H \rightarrow 4 \ell$ for several Higgs boson masses.

Table 1: Higgs boson production cross sections for gluon fusion, vector-boson fusion and associated production with a $W$ or $Z$ boson in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$. The quoted uncertainties correspond to the total theoretical systematic uncertainty. The branching ratio of $H \rightarrow 4 \ell$, with $\ell=e, \mu$, is reported in the last column.

| $m_{H}$ <br> $[\mathrm{GeV}]$ | $\sigma(g g \rightarrow H)$ <br> $[\mathrm{pb}]$ | $\sigma(q q \rightarrow H q q)$ <br> $[\mathrm{pb}]$ | $\sigma(q q \rightarrow W H)$ <br> $[\mathrm{pb}]$ | $\sigma(q q \rightarrow Z H)$ <br> $[\mathrm{pb}]$ | $\mathrm{BR}(H \rightarrow 4 \ell)$ <br> $\cdot 10^{-3}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 130 | $14.1_{-2.1}^{+2.7}$ | $1.154_{-0.027}^{+0.032}$ | $0.501 \pm 0.020$ | $0.278 \pm 0.014$ | 0.19 |
| 150 | $10.5_{-1.6}^{+2.0}$ | $0.962_{-0.021}^{+0.028}$ | $0.300 \pm 0.012$ | $0.171 \pm 0.009$ | 0.38 |
| 200 | $5.2_{-0.8}^{+0.9}$ | $0.637_{-0.015}^{+0.022}$ | $0.103 \pm 0.005$ | $0.061 \pm 0.004$ | 1.15 |
| 300 | $2.4 \pm 0.3$ | $0.301_{-0.008}^{+0.014}$ | $0.020 \pm 0.001$ | $0.012 \pm 0.001$ | 1.38 |
| 400 | $2.0 \pm 0.3$ | $0.162_{-0.005}^{+0.010}$ | - | - | 1.21 |
| 600 | $0.33 \pm 0.06$ | $0.058_{-0.002}^{+0.005}$ | - | - | 1.23 |

The $Z Z^{(*)}$ continuum background is generated using PYTHIA, taking into account $Z-\gamma$ interference. For the inclusive total cross section and the shape of the $m_{Z Z(*)}$ spectrum, the MCFM [50,51] prediction is used, which includes both quark-antiquark annihilation at QCD NLO and gluon fusion. The inclusive
$Z$ boson production, $Z+$ jets, is modelled using ALPGEN [52] and is divided into $Z+$ light-flavour-jets, which includes also $Z c \bar{c}$ at the massless $c$-quark approximation and $Z b \bar{b}$ from parton showers, and $Z b \bar{b}$ using massive matrix elements. The overlaps between the two samples are removed. Specifically, $b \bar{b}$ pairs with separation $\Delta R=\sqrt{(\Delta \phi)^{2}+(\Delta \eta)^{2}} \geq 0.4$ between the $b$-quarks are taken from the matrixelement calculation, whereas for $\Delta R<0.4$ the parton-shower $b \bar{b}$ pairs are taken. PYTHIA is also used as a cross-check of the ALPGEN results. In this search the $Z+$ jets background is normalized using data control samples, but for comparisons the QCD NNLO FEWZ [53,54] and the MCFM [50,51] cross section calculations are used for the inclusive $Z$ boson and $Z b \bar{b}$ production, respectively. The $t \bar{t}$ background is modelled using MC@NLO [55] and is normalized to the approximate NNLO cross section calculated using HATHOR [56]. Both ALPGEN and MC@NLO are interfaced to HERWIG [57] for parton shower hadronization and to JIMMY [58] for the underlying event simulations.

All generated events undergo a full detector simulation performed using GEANT4 [59, 60]. Additional $p p$ interactions in the same bunch crossing (pile-up) are included in the simulation. The MC samples are reweighted to reproduce the observed distribution of the mean number of interactions per bunch crossing in the data.

## 4 Physics Object Identification and Event Selection

The data considered in this analysis were selected using single-lepton triggers. The trigger threshold on the transverse energy, $E_{\mathrm{T}}$, of electrons was $20-22 \mathrm{GeV}$ depending on the LHC instantaneous luminosity, while for muons the $p_{\mathrm{T}}$ threshold was 18 GeV . Both triggers are more than $99.5 \%$ efficient for events passing the offline selection described below.

Electron candidates consist of clusters of energy deposited in the electromagnetic calorimeter associated to ID tracks. The electron candidates must satisfy a set of identification criteria [61], which require the shower profiles to be consistent with those expected for electromagnetic showers and a well reconstructed ID track pointing to the corresponding cluster. The electron transverse momentum is computed from the cluster energy and the track direction at the interaction point.

Muon candidates are reconstructed by matching ID tracks with either full or partial tracks in the MS $[62,63]$. For the former case, the two independent momentum measurements are combined, whereas for the latter case the momentum is measured using the ID information only, with the MS providing muon identification. To reject cosmic rays, muon tracks are required to have a transverse impact parameter with respect to the primary vertex, defined as the reconstructed vertex with the highest $\sum p_{\mathrm{T}}^{2}$ of associated tracks among the reconstructed vertices with at least three associated tracks, of less than 1 mm .

Leptons from Higgs boson decays are expected to be isolated and to originate from the primary vertex. The longitudinal impact parameter of the leptons is required to be within 10 mm from the primary vertex. Track and calorimeter isolation requirements, together with requirements on the transverse impact parameter significance of the lepton, are applied to further reduce the $Z+$ jets and $t \bar{t}$ background contributions. The transverse impact parameter significance of the lepton is defined as its impact parameter in the transverse plane with respect to the primary vertex, divided by the corresponding uncertainty.

The sum of the $p_{\mathrm{T}}$ of tracks within $\Delta R<0.2$ of the lepton divided by the lepton $p_{\mathrm{T}}$ is required to be less than 0.15 , while the sum of the $E_{\mathrm{T}}$ of the calorimeter cells within $\Delta R<0.2$ around the lepton divided by the lepton $p_{\mathrm{T}}$ is required to be less than 0.3 . The track of the lepton candidate and the energies of cells associated to it are excluded from the calculation of the isolation energy. For the calorimeter isolation of electrons, in particular, the transverse energies in the $5 \times 7$ electromagnetic calorimeter cells around the cluster barycenter are excluded [61]. To reduce the impact of pile-up, the tracks included in the $p_{\mathrm{T}}$ sum for track isolation must be associated with the primary vertex, and the transverse energy included in the $E_{\mathrm{T}}$ sum for calorimeter isolation is corrected by subtracting an average offset as a function of the number
of reconstructed vertices in the event. In events with four-lepton invariant mass below 190 GeV , the transverse impact parameter significance for the two lowest $p_{\mathrm{T}}$ leptons in the quadruplet is required to be less than 3.5 and 6 for muons and electrons respectively. The selection efficiency of the isolation and impact parameter requirements has been studied using data both for isolated leptons, with $Z \rightarrow \ell \ell$ decays, and non-isolated leptons from semi-leptonic $b$ and $c$-quark decays in a heavy-flavour enriched dijet sample. Good agreement is observed between data and simulation.

Higgs boson candidates are searched for by selecting two same-flavour, opposite-sign isolated lepton pairs in an event. Each lepton must satisfy $p_{\mathrm{T}}>7 \mathrm{GeV}$ and be measured in the pseudorapidity range $|\eta|<2.47$ for electrons and $|\eta|<2.7$ for muons. At least two leptons in the quadruplet must have $p_{\mathrm{T}}>20 \mathrm{GeV}$. The leptons are required to be well-separated from each other with $\Delta R>0.1$. The invariant mass of the lepton pair closest to the nominal $Z$ boson mass $\left(m_{Z}\right)$ is denoted $m_{12}$ and it is required that $\left|m_{Z}-m_{12}\right|<15 \mathrm{GeV}$. The invariant mass of the remaining, lepton pair, $m_{34}$, is required to be lower than 115 GeV and greater than a threshold depending on the reconstructed four-lepton mass, $m_{4 \ell}$, as summarized in Table 2. The final discriminating variable is $m_{4 \ell}$, where the Higgs boson production would appear as a clustering of events. In Fig. 1 the invariant mass distributions for the $4 \mu$ and $4 e$ channels are presented for a simulated signal sample with $m_{H}=130 \mathrm{GeV}$. The width of the reconstructed Higgs boson mass distribution is dominated by experimental resolution at low $m_{H}$ values, while at high $m_{H}$ the reconstructed width is dominated by the natural width of the Higgs boson with a full-width at half-maximum of approximately 35 GeV at $m_{H}=400 \mathrm{GeV}$.

Table 2: Thresholds applied to $m_{34}$ for reference values of $m_{4 \ell}$ (see text). For other $m_{4 \ell}$ values, the selection requirement is obtained via linear interpolation.

| $m_{4 \ell}(\mathrm{GeV})$ | $\leq 120$ | 130 | 140 | 150 | 160 | 165 | 180 | 190 | $\geq 200$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| threshold $(\mathrm{GeV})$ | 15 | 20 | 25 | 30 | 30 | 35 | 40 | 50 | 60 |

## 5 Background Estimation

The composition of the background is verified in a control region defined by the analysis selection, but without applying the charge, isolation and impact parameter requirements on the second lepton pair. The $m_{34}$ distributions in this control sample are presented in Fig. 2. For large values of $m_{34}$ the $Z Z$ background dominates, while for low values of $m_{34}$ the dominant background source depends on the flavour of the second lepton pair. In final states with a ee second pair, the $Z+$ light-flavour-jets background is dominant, while the $Z b \bar{b}$ production dominates the final states with a $\mu \mu$ second pair. The normalization of the $t \bar{t}$ background, which also contributes substantially in the latter final state, is verified using a control region with opposite-sign electron-muon pairs consistent with the $Z$ boson mass and two additional same-flavour leptons. The $Z Z^{(*)}$ background is normalized using MC, while the $Z+$ jets is normalized using data. The observed background rate, which is found to be in good agreement with expectation, is extrapolated to the signal region by means of the MC simulation.

## 6 Systematic Uncertainties

Uncertainties on lepton reconstruction and identification efficiency, and on the momentum resolution and momentum scale are determined using samples of $W, Z$ and $J / \psi$ decays. The muon efficiency uncertainty results in an acceptance uncertainty on the signal and the irreducible background which is uniform over the mass range of interest and amounts to $0.22 \%(0.16 \%)$ for the $4 \mu(2 e 2 \mu)$ channel. The


Figure 1: Invariant mass distributions for simulated (a) $H \rightarrow Z Z^{(*)} \rightarrow 4 \mu$ (b) $H \rightarrow Z Z^{(*)} \rightarrow 4 e$ for $m_{H}=$ 130 GeV . The fraction of events outside the $\pm 2 \sigma$ region is found to be $15 \%$ for $4 \mu$ and $18 \%$ for $4 e$ for $m_{H}=130 \mathrm{GeV}$.


Figure 2: Invariant mass distribution of the second lepton pair:(a) $\mu \mu$ and (b) $e e$. The kinematic selections of the analysis have been applied. Isolation requirements have been applied on the first lepton pair. No charge requirements were applied to the second lepton pair.
uncertainty on the electron efficiency results in an acceptance uncertainty of $2.3 \%$ ( $1.6 \%$ ) for the $4 e$ $(2 e 2 \mu)$ channel at $m_{4 \ell}=600 \mathrm{GeV}$ and reaching $8.0 \%(4.1 \%)$ at $m_{4 \ell}=110 \mathrm{GeV}$. The effect of the muon momentum resolution and scale uncertainty is found to be small. For electrons the energy resolution uncertainty is relatively small, while the uncertainty on $m_{4 \ell}$ due to the electron energy scale uncertainty
is estimated to be $0.6 \%(0.3 \%)$ for the $4 e(2 e 2 \mu)$ channel. Fitting energy scales to the data can cause fluctuations to align, so to be conservative the energy scale uncertainty is neglected when combining results in the current analysis.

A conservative theoretical uncertainty of $15 \%$ is assigned to the $Z^{(*)}$ background contribution [64]. The $Z+$ light-flavour-jets and $Z b \bar{b}$ backgrounds are evaluated using data. A systematic uncertainty of $45 \%$ and $40 \%$, respectively, is assigned on their normalization to account for the statistical uncertainty in the control sample and the MC-based extrapolation to the signal region. The theoretical uncertainties on the $t \bar{t}$ cross-section, approximately $10 \%$ [56], are included. The additional uncertainty in the $t \bar{t}$ selection efficiency, estimated to be $10 \%$, is negligible in comparison with the errors on the larger backgrounds.

The theoretical uncertainties on the Higgs boson production cross section are 15-20\% for the gluon fusion process, $3-9 \%$ for the vector-boson fusion and $3-4 \%$ for the associated production $(\mathrm{WH} / \mathrm{ZH})$ process [29], depending on the Higgs boson mass. They include uncertainties on the QCD scale and on the parton distribution functions [65-68]. An additional $2 \%$ uncertainty is added to the signal selection efficiency due to the modelling of the signal kinematics. This is evaluated by comparing signal samples generated with PYTHIA and the default POWHEG samples.

The overall uncertainty on the integrated luminosity for the complete 2011 dataset is $3.9 \%$, based on the calibration described in Ref. [18] with an additional uncertainty for the extrapolation to the later data-taking period with higher instantaneous luminosity.

## 7 Results

The number of events observed in each final state, evaluated separately for $m_{4 \ell}<180 \mathrm{GeV}$ and $m_{4 \ell} \geq$ 180 GeV , are compared with the expectations for background and signal for various $m_{H}$ hypotheses in Table 3. In total 71 candidate events are selected by the analysis: $244 \mu, 302 e 2 \mu$, and $174 e$ events, while in the same mass range $62 \pm 9$ events are expected from the background processes; $18.6 \pm 2.84 \mu$, $29.7 \pm 4.52 e 2 \mu$ and $13.4 \pm 2.04 e$. The $m_{12}$ and $m_{34}$ mass spectra are shown in Fig. 3. The $m_{4 \ell}$ distribution for the total background and several signal hypotheses is compared to the data in Fig. 4. In Fig. 5, the $p_{\mathrm{T}}$ and $\eta$ distributions of the leptons of the selected candidates are provided.

Upper limits are set on the Higgs boson production cross section at $95 \%$ CL, using the $C L_{s}$ modified frequentist formalism [69] with the profile likelihood test statistic [70]. The test statistic is evaluated with a maximum likelihood fit of signal and background models to the observed $m_{4 \ell}$ distribution. Figure 6 shows the expected and observed $95 \%$ CL cross section upper limits as a function of $m_{H}$ and Table 4 summarizes the numerical values for selected $m_{H}$ points. The SM Higgs boson is excluded at $95 \%$ CL in the mass ranges $135 \mathrm{GeV}-156 \mathrm{GeV}, 181 \mathrm{GeV}-234 \mathrm{GeV}$ and $255 \mathrm{GeV}-415 \mathrm{GeV}$. The expected exclusion ranges are $137 \mathrm{GeV}-158 \mathrm{GeV}$ and $185 \mathrm{GeV}-400 \mathrm{GeV}$.

The $p_{0}$-value is the probability of upward fluctuations in the background as high as or higher than the excesses observed in data. The consistency of the observed results with the background-only hypothesis expressed as $p_{0}$-values is shown in Fig. 7 over the full mass range of the analysis. The most significant deviations from the background-only hypothesis are observed for $m_{H}=125 \mathrm{GeV}$ with a local $p_{0}$-value of $1.8 \%(2.1 \sigma), m_{H}=244 \mathrm{GeV}$ with a local $p_{0}$-value of $1.1 \%(2.3 \sigma)$ and $m_{H}=500 \mathrm{GeV}$ with a $p_{0}-$ value of $1.4 \%(2.2 \sigma)$. These values do not account for the so-called look-elsewhere effect, taking into account that such an excess (or larger) can appear anywhere in the search range as a result of an upward fluctuation of the background.

For an estimate of the look-elsewhere effect, similarly to Ref. [8], the method of Ref. [71] is used. When considering the complete mass range of this search, the global $p_{0}$-value for all the three excesses becomes more than $50 \%$. In particular for the excess at $m_{H}=125 \mathrm{GeV}$, if the mass range is (a posteriori) constrained to the lowest mass region not excluded at $99 \%$ by the recent LHC combined Higgs search results [8] ( $m_{H}<146 \mathrm{GeV}$ ), the global $p_{0}$-value becomes of $O(30 \%)$. From these it is concluded that,

Table 3: The expected number of signal and background events, with their systematic uncertainty, separated into "Low $m_{4 \ell \text { " }}\left(m_{4 \ell}<180 \mathrm{GeV}\right)$ and "High- $m_{4} \ell$ " $\left(m_{4 \ell} \geq 180 \mathrm{GeV}\right)$ regions. The observed numbers of events are also presented.

|  | $\mu \mu \mu \mu$ |  | ee $\mu \mu$ |  | eeee |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Low $m_{4 \ell}$ | High $m_{4 \ell}$ | Low $m_{4 \ell}$ | High $m_{4 \ell}$ | Low $m_{4 \ell}$ | High $m_{4 \ell}$ |
| Int. Luminosity | $4.81 \mathrm{fb}^{-1}$ | $4.81 \mathrm{fb}^{-1}$ | $4.91 \mathrm{fb}^{-1}$ |  |  |  |
| $Z Z^{(*)}$ | $2.0 \pm 0.3$ | $16.3 \pm 2.4$ | $2.8 \pm 0.6$ | $25.2 \pm 3.8$ | $1.3 \pm 0.3$ | $10.3 \pm 1.5$ |
| $Z, Z b \bar{b}$, and $t \bar{t}$ | $0.16 \pm 0.06$ | $0.02 \pm 0.01$ | $1.4 \pm 0.5$ | $0.17 \pm 0.08$ | $1.6 \pm 0.7$ | $0.18 \pm 0.08$ |
| Total Background | $2.2 \pm 0.3$ | $16.3 \pm 2.4$ | $4.2 \pm 0.8$ | $25.4 \pm 3.8$ | $2.9 \pm 0.8$ | $10.5 \pm 1.5$ |
| Data | 3 | 21 | 3 | 27 | 2 | 15 |
| $m_{H}=125 \mathrm{GeV}$ | $0.58 \pm 0.10$ | $0.73 \pm 0.13$ | $0.25 \pm 0.05$ |  |  |  |
| $m_{H}=130 \mathrm{GeV}$ | $1.00 \pm 0.17$ | $1.22 \pm 0.21$ | $0.43 \pm 0.08$ |  |  |  |
| $m_{H}=150 \mathrm{GeV}$ | $2.1 \pm 0.4$ | $2.9 \pm 0.4$ | $1.12 \pm 0.18$ |  |  |  |
| $m_{H}=200 \mathrm{GeV}$ | $4.9 \pm 0.7$ | $7.7 \pm 1.0$ | $3.1 \pm 0.4$ |  |  |  |
| $m_{H}=300 \mathrm{GeV}$ | $2.9 \pm 0.4$ | $4.9 \pm 0.6$ | $2.1 \pm 0.3$ |  |  |  |
| $m_{H}=400 \mathrm{GeV}$ | $2.0 \pm 0.3$ | $3.3 \pm 0.5$ | $1.49 \pm 0.21$ |  |  |  |
| $m_{H}=600 \mathrm{GeV}$ | $0.34 \pm 0.04$ | $0.62 \pm 0.10$ | $0.30 \pm 0.06$ |  |  |  |



Figure 3: Invariant mass distributions (a) $m_{12}$ and (b) $m_{34}$ for the selected candidates. The data (dots) are compared to the background expectations from the dominant $Z Z^{(*)}$ process and the sum of $t \bar{t}, Z b \bar{b}$ and $Z+$ light-flavour-jets processes. Error bars represent $68.3 \%$ central confidence intervals.
once the look-elsewhere effect is considered, none of the observed local excesses is significant by itself.


Figure 4: $m_{4 \ell}$ distribution of the selected candidates, compared to the background expecation. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown. The resolution of the reconstructed Higgs mass is dominated by detector resolution at low $m_{H}$ values and by the Higgs boson width at high $m_{H}$.


Figure 5: (a) $p_{\mathrm{T}}$ distribution and (b) $\eta$ distribution for the leptons of the 71 candidates surviving the selection criteria. The expected background distributions are also shown. Error bars represent $68.3 \%$ central confidence intervals.

## 8 Summary

A search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ based on $4.8 \mathrm{fb}^{-1}$ of data recorded by the ATLAS detector at $\sqrt{s}=7 \mathrm{TeV}$ during the 2011 run has been presented. The SM


Figure 6: The expected (dashed) and observed (full line) $95 \%$ CL upper limits on the Higgs boson production cross section as a function of the Higgs boson mass, divided by the expected SM Higgs boson cross section. The green and yellow bands indicate the expected sensitivity with $\pm 1 \sigma$ and $\pm 2 \sigma$ fluctuations, respectively.

Table 4: Median expected and observed 95\% CL upper limits on the Higgs boson production cross section for several Higgs boson masses, divided by the expected SM Higgs boson cross section.

| Mass $(\mathrm{GeV})$ | Expected | Observed |
| :---: | :--- | :--- |
| 120 | 5.06 | 5.00 |
| 130 | 1.53 | 1.81 |
| 150 | 0.67 | 0.63 |
| 200 | 0.61 | 0.67 |
| 300 | 0.78 | 0.53 |
| 400 | 1.00 | 0.73 |
| 600 | 4.82 | 8.22 |

Higgs boson is excluded at $95 \%$ confidence level in the mass ranges $135 \mathrm{GeV}-156 \mathrm{GeV}, 181 \mathrm{GeV}-$ 234 GeV and $255 \mathrm{GeV}-415 \mathrm{GeV}$. The largest deviations from the background expectation are observed for $m_{H}=125 \mathrm{GeV}$ with a $p_{0}$-value of $1.8 \%, m_{H}=244 \mathrm{GeV}$ with a $p_{0}$-value of $1.1 \%$ and $m_{H}=500 \mathrm{GeV}$ with a $p_{0}$-value of $1.4 \%$. Once the look-elsewhere effect is considered, none of these excesses is significant by itself.


Figure 7: The consistency of the observed results with the background-only hypothesis expressed as $p_{0}$ values is shown. The dashed line shows the median expected significance in the hypothesis of a Standard Model Higgs boson production. The two horizontal dashed lines indicate the $p_{0}$-values corresponding to local significances of $2 \sigma$ and $3 \sigma$. In (a) the full mass range is presented, while in (b) the low mass range is presented.

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## A Additional Plots



Figure 8: Multiplicity of additional muons with $p_{T}>7 \mathrm{GeV}$ in events with a reconstructed $Z \rightarrow \ell \ell$ decay before and after the subtraction of muons originating from light quarks and $Z Z, W Z$ and $t \bar{t}$ decays. For the cases with two additional muons, their invariant mass is required to be less than 72 GeV . The MC expectation for the heavy flavour component, $Q$, is also presented. The uncertainties shown include both statistical and systematic effects.


Figure 9: Invariant mass distribution of the first lepton pair:(a) $\mu \mu$ and (b) $e e$. The kinematic selections of the analysis have been applied. Isolation requirements have been applied on the first lepton pair. No charge requirements were applied to the second lepton pair.


Figure 10: Event displays of a $4 \mu$ candidate event with $m_{4 \ell}=124.6 \mathrm{GeV}$. The masses of the lepton pairs are 89.7 GeV and 24.6 GeV .


Figure 11: Event displays of a $2 e 2 \mu$ candidate event with $m_{4 \ell}=124.3 \mathrm{GeV}$. The masses of the lepton pairs are 76.8 and 45.7 GeV .


Figure 12: Event display of a $2 \mu 2 e$ candidate event with $m_{4 \ell}=123.6 \mathrm{GeV}$. The masses of the lepton pairs are 89.3 and 30.0 GeV .

## ATLAS NOTE

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# Search for high-mass dilepton resonances with $5 \mathbf{f b}^{-1}$ of $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS experiment 

The ATLAS Collaboration


#### Abstract

This note reports on a search for narrow high-mass resonances decaying into dilepton final states. The data, recorded by the ATLAS experiment in $p p$ collisions at $\sqrt{s}=7 \mathrm{TeV}$ at the Large Hadron Collider, correspond to a total integrated luminosity of $4.9(5.0) \mathrm{fb}^{-1}$ in the $e^{+} e^{-}\left(\mu^{+} \mu^{-}\right)$channel. No statistically significant excess above the Standard Model expectation is observed, and upper limits are set at the $95 \%$ confidence level on the cross section times branching fraction of $Z^{\prime}$ resonances and Randall-Sundrum gravitons decaying into dileptons as a function of the resonance mass. A lower limit of 2.21 TeV on the mass of the Sequential Standard Model $Z^{\prime}$ boson is set. A Randall-Sundrum graviton with coupling $k / \bar{M}_{\mathrm{Pl}}=0.1$ is excluded at $95 \%$ confidence level for masses below 2.16 TeV .


## 1 Introduction

This note describes a search for narrow high-mass resonances decaying into $e^{+} e^{-}$or $\mu^{+} \mu^{-}$pairs using $7 \mathrm{TeV} p p$ collision data recorded with the ATLAS detector [1] at the Large Hadron Collider (LHC). Such resonances, which are predicted by several extensions of the Standard Model (SM), include new heavy spin-1 neutral gauge bosons such as $Z^{\prime}[2,3,4]$ and $Z^{*}$ [5], techni-mesons $[6,7,8]$, as well as spin-2 Randall-Sundrum gravitons, $G^{*}$ [9].

The benchmark models considered for the $Z^{\prime}$ are the Sequential Standard Model (SSM) [3], with the same couplings to fermions as the $Z$ boson, and the $\mathrm{E}_{6}$ Grand Unified symmetry group [2], broken into $\operatorname{SU}(5)$ and two additional $\mathrm{U}(1)$ groups, leading to new neutral gauge fields $\psi$ and $\chi$. The particles associated with the additional fields can mix in a linear combination to form the $Z^{\prime}$ candidate: $Z^{\prime}\left(\theta_{E_{6}}\right)=$ $Z_{\psi}^{\prime} \cos \theta_{E_{6}}+Z_{\chi}^{\prime} \sin \theta_{E_{6}}$, where $\theta_{E_{6}}$ is the mixing angle between the two gauge bosons. The pattern of spontaneous symmetry breaking and the value of $\theta_{E_{6}}$ determine the $Z^{\prime}$ couplings to fermions; six choices of $\theta_{E_{6}}[2,3]$ lead to the specific $Z^{\prime}$ states named $Z_{\psi}^{\prime}, Z_{N}^{\prime}, Z_{\eta}^{\prime}, Z_{I}^{\prime}, Z_{S}^{\prime}$ and $Z_{\chi}^{\prime}$.

Other models predict additional spatial dimensions as a possible explanation for the gap between the electroweak symmetry breaking scale and the gravitational energy scale. The Randall-Sundrum (RS) model [9] predicts excited Kaluza-Klein modes of the graviton, which appear as spin-2 resonances. These modes have a narrow intrinsic width when $k / \bar{M}_{\mathrm{Pl}}<0.1$, where $k$ is the spacetime curvature in the extra dimension, and $\bar{M}_{\mathrm{Pl}}=M_{\mathrm{Pl}} / \sqrt{8 \pi}$ is the reduced Planck scale.

Previous searches have set direct and indirect constraints on the mass of the $Z^{\prime}$ and $G^{*}$ resonances [10, 11]. The Tevatron experiments [12, 13] excluded a $Z_{\text {SSM }}^{\prime}$ with a mass lower than 1.071 TeV [13]. Recent measurements by the ATLAS and CMS collaborations based on $1 \mathrm{fb}^{-1}$ of data excluded a $Z_{\text {SSM }}^{\prime}$ with a mass lower than 1.83 TeV [14] and 1.94 TeV [15], respectively. In addition, indirect constraints from LEP [16, 17, 18, 19] have set a limit of 1.787 TeV [11] on the $Z_{\text {SSM }}^{\prime}$. Constraints on the mass of the RS graviton have been set by the ATLAS [14, 20], CMS [15, 21], CDF [22] and D0 [23] collaborations. Assuming $k / \bar{M}_{\mathrm{Pl}}=0.1, \mathrm{CDF}$ and D 0 excluded graviton masses below 1.058 TeV and 1.050 TeV respectively, with the dielectron and diphoton channels combined; CMS excluded masses below 1.84 TeV with the diphoton channel only using $2 \mathrm{fb}^{-1}$ of data, and masses below 1.78 TeV with the dielectron plus dimuon channels using $1 \mathrm{fb}^{-1}$ of data; the ATLAS lower limit was 1.95 TeV with the combination of the dielectron and dimuon channels (using $1 \mathrm{fb}^{-1}$ of data) and of the diphoton channel (using $2 \mathrm{fb}^{-1}$ of data).

## 2 ATLAS detector, data selection and trigger

The ATLAS detector consists of an inner detector surrounded by a 2 T superconducting solenoid, electromagnetic and hadronic calorimeters, and a muon spectrometer with a toroidal magnetic field. Charged particle tracks in the pseudorapidity ${ }^{1}$ range $|\eta|<2.5$ are reconstructed with the inner detector, which consists of silicon pixel, silicon strip, and transition radiation detectors. The superconducting solenoid is surrounded by a hermetic calorimeter that covers $|\eta|<4.9$. For $|\eta|<2.5$, the electromagnetic calorimeter is finely segmented and plays an important role in electron identification. Outside the calorimeter, aircore toroids provide the magnetic field for the muon spectrometer. Three stations of precision drift tubes (with cathode strip chambers for the innermost station for $|\eta|>2.0$ ) provide an accurate measurement of the muon track curvature in the range $|\eta|<2.7$. Resistive-plate and thin-gap chambers provide muon triggering capability in the range $|\eta|<2.4$.

The data sample used in this analysis, recorded during 2011, corresponds to a total integrated luminosity of $4.9(5.0) \mathrm{fb}^{-1}$ in the dielectron (dimuon) channel. The trigger used in the electron channel

[^68]requires at least two electromagnetic clusters in the calorimeter, each with a transverse energy of at least 20 GeV . It was measured in data to be $99 \%$ efficient with respect to the event selection described below for dilepton masses above 100 GeV . For the muon channel, the trigger requires the presence of a single muon with a transverse momentum ( $p_{\mathrm{T}}$ ) threshold of 22 GeV ; the single-muon trigger efficiency was measured in data to be $85 \%$ in the barrel for most of the data-taking period, and $86 \%$ in the endcaps for the entire dataset. The muon trigger efficiency is lower than the electron trigger efficiency because of the lower geometrical acceptance of the muon trigger detectors.

## 3 Event selection

The triggered events are required to have a primary vertex with at least three associated charged particle tracks with $p_{\mathrm{T}}>0.4 \mathrm{GeV}$.

In the dielectron channel, two electron candidates are required with transverse energy $E_{\mathrm{T}}>25 \mathrm{GeV}$ and $|\eta|<2.47$; the transition region $1.37 \leq|\eta| \leq 1.52$ between the barrel and the endcap calorimeters is excluded. Electron candidates are formed from clusters of cells reconstructed in the electromagnetic calorimeter associated with a charged particle track in the inner detector. Criteria on the transverse shower shape, the longitudinal leakage into the hadronic calorimeter, and the association with an inner detector track are applied to the cluster to define a so-called Medium electron [24]. The electron energy is obtained from the calorimeter measurement and its direction from the associated track. The calorimeter energy resolution is dominated at large $E_{\mathrm{T}}$ by a constant term which is $1.2 \%$ in the barrel and $1.8 \%$ in the endcaps. A hit in the first active pixel layer is required to suppress background from photon conversions. To further suppress background from QCD multijet production, the higher $E_{\mathrm{T}}$ electron must be isolated, requiring that $\Sigma E_{\mathrm{T}}(\Delta R<0.2)<7 \mathrm{GeV}$, where $\Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}$ and $\Sigma E_{\mathrm{T}}(\Delta R<0.2)$ is the sum of the transverse energy deposition in the calorimeter around the electron direction. The core of the electron energy deposition is excluded and the sum is corrected for transverse shower leakage and pile-up from additional $p p$ collisions. Since the resolution on the dielectron mass is dominated by the calorimeter energy measurements, the two electron candidates are not required to have opposite charge, which to minimizes the losses due to charge mis-identification. For these selection criteria, the total signal acceptance for a $Z^{\prime} \rightarrow e^{+} e^{-}\left(G^{*} \rightarrow e^{+} e^{-}\right)$of mass 2 TeV is $71 \%$ ( $72 \%$ ), approximately independent of mass above 600 GeV . These numbers account for the acceptance of all selection criteria and efficiencies, and reflect the differences in lepton angular distributions due to spin.

In the dimuon channel, two muon candidates of opposite charge are required, each satisfying $p_{\mathrm{T}}>$ 25 GeV . Muon tracks are reconstructed independently in both the inner detector and muon spectrometer, and their momenta are determined from a combined fit to these two measurements. To optimize the momentum resolution, each muon candidate is required to pass quality cuts in both the inner detector and the muon spectrometer. Most muons used in the analysis have at least three hits in each of the inner, middle, and outer layers of the muon spectrometer. To increase the reconstruction efficiency, muons reconstructed in only two layers of the muon spectrometer are also included in the search if they are in regions where the toroidal field is strong and the detector well aligned. Muons with hits in both the barrel and the endcap regions are discarded because of residual misalignment between these two parts of the muon spectrometer. The effects of misalignments and intrinsic position resolution are included in the simulation by applying a smearing to $q / p_{\mathrm{T}}$, which reproduces the momentum resolution of the data. The $p_{\mathrm{T}}$ resolution at 1 TeV for muons reconstructed combining the measurements in the inner detector and muon spectrometer ranges from about $10 \%$ to $25 \%$.

To suppress background from cosmic rays, the $z$ position of the primary vertex is required to be within 200 mm of the centre of the detector, and the muon tracks are required to have a transverse impact parameter $\left|d_{0}\right|<0.2 \mathrm{~mm}$ and a distance along the beam-line to the primary vertex below 1 mm . To reduce background from jets, each muon is required to be isolated such that $\Sigma p_{\mathrm{T}}(\Delta R<0.3) / p_{\mathrm{T}}(\mu)<0.05$,
where only tracks with $p_{\mathrm{T}}>1 \mathrm{GeV}$, and not the muon track, enter the sum. The total signal acceptance is $43 \%(47 \%)$ for a $Z^{\prime} \rightarrow \mu^{+} \mu^{-}\left(G^{*} \rightarrow \mu^{+} \mu^{-}\right)$of mass 2 TeV , including $4 \%$ from events with one muon reconstructed in only two layers of the muon spectrometer. The lower acceptance compared to the electron channel is due to the stringent requirements on the muon selection criteria to improve the $p_{\mathrm{T}}$ resolution.

## 4 Signal and background simulation

For both channels, the dominant and irreducible background is due to the $Z / \gamma^{*}$ (Drell-Yan) process, characterized by the same final state as the signal. Small contributions from $t \bar{t}$ and diboson ( $W W, W Z$ and $Z Z$ ) production are also present in both channels. Semileptonic decays of $b$ and $c$ quarks in the dimuon sample and a mixture of photon conversions, semileptonic heavy quark decays, and hadrons misidentified as electrons in the $e^{+} e^{-}$sample are backgrounds that are referred to below as QCD background or QCD multijet. Jets accompanying $W$ bosons ( $W+$ jets) may similarly produce lepton candidates in addition to the one from $W \rightarrow \ell v$ decay.

The expected signal and backgrounds, with the exception of the QCD multijet background, are evaluated with simulated samples and rescaled using the most precise available cross-section predictions. The $Z^{\prime}, G^{*}$ signal and $Z / \gamma^{*}$ processes are generated with Pythia 6.425 [25] using MRST2007lomod [26] parton distribution functions (PDFs). Interference between the $Z / \gamma^{*}$ process and the $Z^{\prime}$ resonance is expected to be small and therefore neglected. The diboson processes are generated with HERWIG 6.510 [27] using MRST2007lomod PDFs. The $W+$ jets background is generated with ALPGEN [28] using CTEQ6L1 [29] PDFs and the $t \bar{t}$ background with MC@NLO 3.41 [30] using CTEQ66 [31] PDFs. JIMMY 4.31 [32] is used for both processes to describe multiple parton interactions and HERWIG to describe the remaining underlying event and parton showers. Final-state photon radiation is handled with PHOTOS [33]. The samples are processed through a full ATLAS detector simulation [34] based on GEANT4 [35].

The $Z / \gamma^{*}$ cross section is calculated at next-to-next-to-leading order (NNLO) using PHOZPR [36] with MSTW2008 PDFs [37]. The ratio of this cross section to the leading-order cross section is used to determine a mass-dependent QCD K-factor which is applied to the results of the leading-order simulations. The same QCD K-factor is applied to the $Z^{\prime}$ signal. It is 0.91 at 2 TeV and slowly increases towards lower masses. A different K-factor is applied to the $G^{*}$ signal. The calculated values vary between 1.6 and 1.8 , depending on the graviton mass and on $k / \bar{M}_{\mathrm{Pl}}$ [38]; in practice, 1.75 is used above 750 GeV . Electroweak corrections including virtual heavy gauge-boson loops are calculated using HORACE [39, 40], yielding an effective electroweak K-factor which is only applied to the Drell-Yan background.

The $t \bar{t}$ cross section is predicted at approximately NNLO, with $10 \%$ uncertainty [41, 42]. The diboson cross sections are calculated at next-to-leading order (NLO) using MCFM [43]; the $W$ inclusive cross section from ALPGEN, including all possible final states with and without jets, is renormalised to the NNLO calculation of FEWZ [44]; these cross sections are assigned a $5 \%$ uncertainty each, from scale, PDF and $\alpha_{s}$ variations. In the dimuon channel, the $W+$ jets Monte Carlo yield is assigned an overall $30 \%$ systematic uncertainty from the sum of the cross sections of the ALPGEN samples with at least one parton with $E_{\mathrm{T}}>20 \mathrm{GeV}$ accompanying the $W$ boson. In the electron channel, this uncertainty is replaced by a data-driven uncertainty, as explained below.

The QCD multijet background in the dielectron sample is estimated from data using a "reversed electron identification" technique. Data with both electron candidates failing a subset of identification criteria (chosen not to affect kinematic distributions) are used to determine the QCD background distribution versus $m_{e e}$. Contributions from other backgrounds are estimated from simulated samples and subtracted. An empirical function, $f(x)=p_{1} x^{p_{2}+p_{3} \log x}$, fitted in the $110-800 \mathrm{GeV}$ range, extrapolates the distribution to high $m_{e e}$. This QCD background shape and the sum of the $Z / \gamma^{*}$, diboson, $t \bar{t}$ and $W+$ jets backgrounds are fitted to the observed $m_{e e}$ distribution in a control region to determine the
normalization of the QCD contribution. This method provides the central QCD multijet estimate, and two other techniques are used to assign a systematic uncertainty. One is another shape-fitting procedure, this time on two-dimensional (leading and sub-leading electron) isolation distributions in bins of $m_{e e}$. A third independent data-driven QCD multijet estimate is based on fake rates computed from jet-enriched samples obtained from jet triggers or from the electromagnetic-cluster trigger used for the signal. These estimates are compatible with the central method. Since these alternative methods provide combined estimates of the QCD and $W+$ jets contributions, the central QCD multijet determination is summed with the Monte Carlo predicted $W+$ jets yield for the comparison. The largest difference with the alternative methods is assigned as the global systematic uncertainty to the QCD plus $W+$ jets yield in the dielectron channel.

The QCD background in the dimuon sample is evaluated from data using the reversed isolation method described in [45], based on the track isolation variable $\Sigma p_{\mathrm{T}}(\Delta R<0.3) / p_{\mathrm{T}}$.

The QCD and $W+$ jets backgrounds are small for the electron channel and very small for the muon channel. Backgrounds from cosmic rays are negligible.

## 5 Results

The observed invariant mass distributions are compared to the SM expectation, given by the Monte Carlo simulation for all components except QCD multijet, which is taken from the data. For this purpose, the Drell-Yan, $t \bar{t}$, diboson and $W+$ jets backgrounds from Monte Carlo simulation are scaled according to their respective cross sections and added to the data-driven QCD background. The simulated backgrounds are then rescaled so that the sum matches the observed number of data events in the normalization region, defined as the $70-110 \mathrm{GeV}$ mass interval. The scaling factor is within $1.6 \%$ of unity. The number of events in the normalization region is 1237292 in the dielectron channel, and 985004 in the dimuon channel; the Drell-Yan component amounts to more than $99 \%$ of the total in both cases. The advantage of this approach is that the uncertainty on the integrated luminosity, and any mass-independent uncertainties on efficiencies, cancel between the $Z^{\prime}\left(G^{*}\right)$ and the $Z$ boson in the limit computation presented below.

Table 1: The expected and observed numbers of events in the dielectron channel for various $m_{e e}$ bins. The expected numbers are shown separately for each of the background components discussed in the text. The errors quoted include both statistical and systematic uncertainties.

| $m_{e^{+} e^{-}}[\mathrm{GeV}]$ | $110-200$ | $200-400$ | $400-800$ | $800-1200$ | $1200-3000$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{Z} / \gamma^{*}$ | $26300 \pm 800$ | $3080 \pm 120$ | $265 \pm 14$ | $12.2 \pm 0.9$ | $1.46 \pm 0.18$ |
| $t \bar{l}$ | $1300 \pm 70$ | $403 \pm 26$ | $28 \pm 4$ | $1.0 \pm 0.8$ | $0.021 \pm 0.021$ |
| Diboson | $440 \pm 17$ | $147 \pm 8$ | $14.7 \pm 2.2$ | $1.0 \pm 0.4$ | $0.06 \pm 0.06$ |
| $(W+$ jets $)$ and QCD | $2000 \pm 400$ | $420 \pm 160$ | $40 \pm 40$ | $1.8 \pm 1.2$ | $0.11 \pm 0.08$ |
| Total | $30000 \pm 900$ | $4050 \pm 200$ | $340 \pm 40$ | $16.0 \pm 1.8$ | $1.64 \pm 0.21$ |
| Data | 29993 | 4038 | 358 | 17 | 3 |

Figure 1 presents the invariant mass ( $m_{\ell \ell}$ ) distribution for the dielectron (top) and dimuon (bottom) final states after final selection. Figure 1 also displays the expected $Z_{S S M}^{\prime}$ signal for three mass hypotheses. Tables 1 and 2 show the number of data events and the estimated backgrounds in bins of reconstructed dielectron and dimuon invariant mass above 110 GeV . The dilepton invariant mass distributions are well

Table 2: The expected and observed numbers of events in the dimuon channel for various $m_{\mu^{+} \mu^{-}}$bins. The expected numbers are shown separately for each of the background components discussed in the text. The errors quoted include both statistical and systematic uncertainties.

| $m_{\mu^{+} \mu^{-}}[\mathrm{GeV}]$ | $110-200$ | $200-400$ | $400-800$ | $800-1200$ | $1200-3000$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{Z} / \gamma^{*}$ | $21000 \pm 900$ | $2040 \pm 90$ | $174 \pm 9$ | $7.3 \pm 0.5$ | $0.90 \pm 0.11$ |
| $\bar{t}$ | $830 \pm 80$ | $254 \pm 24$ | $20.0 \pm 2.1$ | $0.59 \pm 0.15$ | $<0.005$ |
| Diboson | $283 \pm 15$ | $98 \pm 5$ | $12.7 \pm 1.0$ | $0.83 \pm 0.24$ | $0.022 \pm 0.028$ |
| $(W+$ jets $)$ and QCD | $7 \pm 4$ | $<0.5$ | $<0.5$ | $<0.05$ | $<0.005$ |
| Total | $22100 \pm 900$ | $2400 \pm 90$ | $206 \pm 9$ | $8.7 \pm 0.6$ | $0.92 \pm 0.11$ |
| Data | 21941 | 2293 | 197 | 10 | 2 |

described by the prediction from SM processes.
The invariant mass distribution of the data is compared to templates of the background and of signals with pole masses in the search region, which extends from 0.13 to 3.0 TeV [14, 45]. A likelihood function is defined as the product of the Poisson probabilities over all mass bins in the search region. The Poisson probability in each bin is evaluated for the observed number of data events given the background and signal template expectation. The total signal acceptance as a function of mass is propagated into the expectation, and systematic uncertainties are incorporated in the likelihood via nuisance parameters [46].

The significance of a signal is summarized by a $p$-value, the probability of observing an excess at least as signal-like as the one observed in data, in the absence of signal. The outcome of the search is ranked against pseudo-experiments using a likelihood ratio, which is scanned as a function of $Z^{\prime}$ cross section and $m_{Z^{\prime}}$ over the full considered mass range. The data are consistent with the SM hypothesis, with global $p$-values of $13 \%$ and $82 \%$ for the dielectron and dimuon channels respectively.

In addition, the agreement between data and expectation is studied by computing the significance of the difference in each mass bin, with statistical and systematic errors taken into account [47]; the result is displayed in Figure 2. The largest positive local significance is $\sim 2.5 \sigma$ in the electron channel and less than $2 \sigma$ in the muon channel, and the largest negative significance is about $-3 \sigma$ in both channels.

Given the absence of any significant signal, an upper limit on the number of signal events is determined at the $95 \%$ confidence level (C.L.) using a Bayesian approach [46] with a flat, positive prior on the signal cross section.

## 6 Systematic uncertainties

Systematic uncertainties include the normalization to the $Z$-peak, PDF, QCD and electroweak corrections, as well as the trigger, reconstruction and identification efficiencies. For each source of uncertainty, the correlations across bins, as well as the correlations between signal and background, are taken into account.

Since the total background is normalized to the data in the region of the $Z \rightarrow \ell^{+} \ell^{-}$mass peak, the residual systematic uncertainties (with the exception of the $Z$ cross section uncertainty) are small at the $Z$ pole and grow at higher mass. The dominant uncertainties are theoretical. The overall uncertainty due to $\mathrm{PDF}, \alpha_{S}$, and scale variations is estimated to be $20 \%$ at 2 TeV , where the PDF contribution is dominant. The $\alpha_{S}$ and PDF uncertainties are evaluated using the MSTW2008NNLO eigenvector PDF sets and the PDF sets corresponding to variations of $\alpha_{S}$, at the $90 \%$ C.L. The spread of the variations covers the


Figure 1: The dielectron (top) and dimuon (bottom) invariant mass ( $m_{\ell \ell}$ ) distribution after final selection, compared to the stacked sum of all expected backgrounds, with three example $Z_{\mathrm{SSM}}^{\prime}$ signals overlaid. The bin width is constant in $\log m_{\ell \ell}$.


Figure 2: The dielectron (left) and dimuon (right) invariant mass ( $m_{\ell \ell}$ ) distributions after final selection, compared to the expected background. The bin width is the same as in Figure 1. The bottom part of each histogram shows the significance of the difference between data and expectation in each bin.
difference between the central values obtained with the CTEQ and MSTW PDF sets. The scale uncertainties are estimated by varying the renormalization $\left(\mu_{R}\right)$ and factorization $\left(\mu_{F}\right)$ scales independently up and down by a factor of two, but with the constraint $0.5 \leq \mu_{F} / \mu_{R} \leq 2$. The resulting maximum variations are taken as the uncertainties. Additionally, a systematic uncertainty of $4.5 \%$ is attributed to electroweak corrections [45].

The uncertainty on the $Z / \gamma^{*}$ cross section is $5 \%$, which is applied as a systematic uncertainty on the signal yield. It replaces the uncertainty on the integrated luminosity due to the normalization to the data under the $Z \rightarrow \ell^{+} \ell^{-}$mass peak.

The experimental systematic effects due to resolution and inefficiencies at high mass were also studied. The uncertainty on the energy resolution is measured to be negligible in the electron channel. In the muon channel, the uncertainty on the momentum resolution is due to residual misalignments and intrinsic position uncertainties in the muon spectrometer that propagate to a change in the observed width of the $Z^{\prime}\left(G^{*}\right)$ line-shape. The simulation was adjusted to reproduce the data at high muon momentum. The residual uncertainty translates into an event yield uncertainty of less than $3 \%$. The combined uncertainty on the muon trigger and reconstruction efficiency is estimated to be $6 \%$ at 2 TeV . This uncertainty is dominated by a conservative estimate of the impact of large energy loss from muon bremsstrablung in the calorimeter on the muon reconstruction performance in the muon spectrometer. In the electron channel, a systematic uncertainty of $2 \%$ at 2 TeV is estimated for a possible identification inefficiency caused by the isolation requirement.

The dominant systematic uncertainties are summarized in Table 3. Uncertainties of $3 \%$ and less are neglected in the limit setting procedure described below, and no theory uncertainties are applied to the $Z^{\prime}$ or $G^{*}$ signal.

## 7 Interpretation

The limit on the number of produced $Z^{\prime}\left(G^{*}\right)$ events is converted into a limit on cross section times branching fraction $\sigma B$ by scaling with the observed number of $Z$ boson events and the theoretical value

Table 3: Summary of systematic uncertainties on the expected numbers of events at $m_{\ell^{+} \ell^{-}}=2 \mathrm{TeV}$. NA indicates that the uncertainty is not applicable, and "-" denotes a negligible entry.

| Source | Dielectrons |  | Dimuons |  |
| :--- | :---: | :---: | :---: | :---: |
|  | Signal | Background | Signal | Background |
| Normalization | $5 \%$ | NA | $5 \%$ | NA |
| PDF/ $\alpha_{s} /$ scale | NA | $20 \%$ | NA | $20 \%$ |
| Electroweak corrections | NA | $4.5 \%$ | NA | $4.5 \%$ |
| Efficiency | - | - | $6 \%$ | $6 \%$ |
| $W+$ jets and QCD background | NA | $3.5 \%$ | NA | - |
| Total | $5 \%$ | $21 \%$ | $8 \%$ | $21 \%$ |



Figure 3: The expected and observed 95\% C.L. upper limits on $\sigma B$ as a function of mass for $Z^{\prime}$ (left) and $G^{*}$ (right) models for the electron channel. The thickness of the $Z_{\mathrm{SSM}}^{\prime}$ (left) and the $G^{*}$ for $k / \bar{M}_{\mathrm{Pl}}=0.1$ (right) theory curves illustrate the theoretical uncertainties.
of $\sigma B(Z \rightarrow l l)$. The expected exclusion limits are determined using pseudo-experiments containing only SM processes, by evaluating the $95 \%$ C.L. upper limits for each pseudo-experiment for each fixed value of $m_{Z^{\prime}}\left(m_{G^{*}}\right)$. The median of the distribution of limits represents the expected limit. The ensemble of limits is used to find the $68 \%$ and $95 \%$ envelopes of the expected limits as a function of $m_{Z^{\prime}}\left(m_{G^{*}}\right)$.

Figure 3 shows the $95 \%$ C.L. observed and expected exclusion limits on $\sigma B\left(Z^{\prime} \rightarrow e^{+} e^{-}\right)$and on $\sigma B\left(G^{*} \rightarrow e^{+} e^{-}\right)$. It also shows the theoretical cross section times branching fraction for the $Z_{\mathrm{SSM}}^{\prime}$ and for $\mathrm{E}_{6}$-motivated $Z^{\prime}$ models with the lowest and highest $\sigma B$. The same information is shown in Figure 4 for the muon channel. Figure 5 shows the combined dielectron and dimuon $95 \%$ C.L. observed and expected exclusion limits on $\sigma B\left(Z^{\prime} \rightarrow l l\right)$ and on $\sigma B\left(G^{*} \rightarrow l l\right)$.

Figure 6 shows the ratio between the observed limit and the expected cross section times branching fraction as a function of the $Z^{\prime}$ mass for the SSM model, for previous results at the Tevatron and in ATLAS, together with the results presented here. Mass limits obtained for the $Z_{\mathrm{SSM}}^{\prime}$ and $G^{*}$ (with $k / \bar{M}_{\mathrm{Pl}}=0.1$ ) are displayed in Table 4. The combined mass limits on the $\mathrm{E}_{6}$-motivated models and the $G^{*}$ with various couplings are given in Table 5.

Figures 7 and 8 show event displays of the dielectron and dimuon candidates reconstructed with the highest invariant mass.


Figure 4: The expected and observed $95 \%$ C.L. upper limits on $\sigma B$ as a function of mass for $Z^{\prime}$ (left) and $G^{*}$ (right) models for the muon channel. The thickness of the $Z_{\mathrm{SSM}}^{\prime}$ (left) and the $G^{*}$ for $k / \bar{M}_{\mathrm{P} 1}=0.1$ (right) theory curves illustrate the theoretical uncertainties.

Table 4: The observed (expected) $95 \%$ C.L. mass lower limits in TeV on $Z_{\text {SSM }}^{\prime}$ resonance and $G^{*}$ graviton (with $k / \bar{M}_{\mathrm{P}}=0.1$ ), for the dielectron and dimuon channels separately and for their combination.

| Model | Mass limit [TeV] |  |  |
| :--- | :---: | :---: | :---: |
|  | $e^{+} e^{-}$ | $\mu^{+} \mu^{-}$ | $\ell^{+} \ell^{-}$ |
| $Z_{\text {SSM }}^{\prime}$ | $2.07(2.14)$ | $1.99(2.01)$ | $2.21(2.26)$ |
| $G^{*}$ | $2.03(2.05)$ | $1.90(1.92)$ | $2.16(2.17)$ |

Table 5: The observed $95 \%$ C.L. lower limits on the masses of $\mathrm{E}_{6}$-motivated $Z^{\prime}$ bosons and RS gravitons $G^{*}$ for various values of the coupling $k / \bar{M}_{\mathrm{Pl}}$. Both lepton channels are combined.

|  | $\mathrm{E}_{6} Z^{\prime}$ models |  |  |  |  |  | RS graviton |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Model/Coupling | $Z_{\psi}^{\prime}$ | $Z_{N}^{\prime}$ | $Z_{\eta}^{\prime}$ | $Z_{I}^{\prime}$ | $Z_{S}^{\prime}$ | $Z_{\chi}^{\prime}$ | 0.01 | 0.03 | 0.05 |  |
| Mass limit [TeV] | 1.76 | 1.78 | 1.84 | 1.84 | 1.90 | 1.96 | 0.91 | 1.45 | 1.71 |  |

## 8 Conclusion

The ATLAS detector has been used to search for narrow, high-mass resonances in the dilepton invariant mass spectrum. Proton-proton collision data with integrated luminosities of $4.9(5.0) \mathrm{fb}^{-1}$ in the dielectron (dimuon) channel have been used. The observed invariant mass spectra are consistent with the SM expectations. Limits are set on the cross section times branching fraction $\sigma B$. The resulting lower limits on the mass of a new resonance are 2.21 TeV for a Sequential Standard Model $Z^{\prime}, 1.76-1.96 \mathrm{TeV}$ for various $\mathrm{E}_{6}$-motivated $Z^{\prime}$ bosons and $0.91 \mathrm{TeV}-2.16 \mathrm{TeV}$ for a Randall-Sundrum graviton with couplings $\left(k / \bar{M}_{\mathrm{PI}}\right)$ in the range $0.01-0.1$.


Figure 5: The expected and observed $95 \%$ C.L. upper limits on $\sigma B$ as a function of mass for $Z^{\prime}$ (top) and $G^{*}$ (bottom) models. Both results show the combination of the electron and muon channels. The thickness of the $Z_{\mathrm{SSM}}^{\prime}$ (top) and the $G^{*}$ for $k / \bar{M}_{\mathrm{Pl}}=0.1$ (bottom) theory curves illustrate the theoretical uncertainties.


Figure 6: The ratio between the observed limit and the predicted cross section times branching ratio as a function of the $Z^{\prime}$ mass for the SSM model. The results are shown for the most recent limits from the Tevatron [13, 12], the latest ATLAS published data [14] and the analysis presented here. No uncertainties on the theoretical prediction are applied.

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Figure 7: Event display for the dielectron candidate with the highest reconstructed invariant mass ( $m_{e e}=1.66 \mathrm{TeV}$ ). Both electrons are in the calorimeter end-caps; their tracks are shown in green. The electron with highest transverse energy has an $E_{\mathrm{T}}$ of 329 GeV and an $(\eta, \phi)$ of $(2.00,1.02)$. The subleading electron has an $E_{\mathrm{T}}$ of 217 GeV and an $(\eta, \phi)$ of ( $-1.60,-1.83$ ). The event missing transverse energy is 26 GeV .


Figure 8: Event display for the dimuon candidate with the highest reconstructed invariant mass $\left(m_{\mu \mu}=1.25 \mathrm{TeV}\right)$. The muon with highest momentum has a $p_{\mathrm{T}}$ of 648 GeV and an $(\eta, \phi)$ of $(-0.75,0.49)$. The subleading muon has a $p_{\mathrm{T}}$ of 583 GeV and an $(\eta, \phi)$ of $(-0.36,-2.60)$. The event missing transverse energy is 67 GeV , with a $\phi_{M E T}$ of -2.83 .
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ATLAS NOTE
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# Observation of an excess of events in the search for the Standard Model Higgs boson in the $H \rightarrow Z Z Z^{(*)} \rightarrow 4 \ell$ channel with the ATLAS detector 

The ATLAS Collaboration


#### Abstract

This note presents a search for the Standard Model Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{\prime}+\ell^{\prime}$, where $\ell, \ell^{\prime}=e$ or $\mu$, using $4.8 \mathrm{fb}^{-1}$ and $5.8 \mathrm{fb}^{-1}$ of proton-proton collisions at $\sqrt{s}=7 \mathrm{TeV}$ and 8 TeV , respectively, recorded with the ATLAS detector. The four-lepton invariant mass distribution is compared with Standard Model background expectations to derive upper limits on the cross section of a Standard Model Higgs boson with a mass between 110 GeV and 600 GeV . The mass ranges $131-162 \mathrm{GeV}$ and $170-$ 460 GeV are excluded at the $95 \%$ confidence level, while the expected exclusion ranges at the $95 \%$ confidence level are $124-164 \mathrm{GeV}$ and $176-500 \mathrm{GeV}$. An excess of events is observed around $m_{H}=125 \mathrm{GeV}$, whose local $p_{0}$ value is $0.029 \%$ ( 3.4 standard deviations) in the combined analysis of the two datasets.


## 1 Introduction

The Higgs mechanism in the context of the Standard Model (SM) is the source of electroweak symmetry breaking and results in the appearance of the Higgs boson [1-3], which remains the only unobserved particle of the Standard Model. Direct searches performed at the CERN Large Electron-Positron Collider (LEP) excluded at $95 \%$ confidence level (CL) the production of a SM Higgs boson with mass, $m_{H}$, less than 114.4 GeV [4]. The searches at the Fermilab Tevatron $p \bar{p}$ collider have excluded at $95 \%$ CL the region $147 \mathrm{GeV}<m_{H}<179 \mathrm{GeV}$ [5]. At the LHC, the ATLAS experiment using $4.9 \mathrm{fb}^{-1}$ of data at $\sqrt{s}=7 \mathrm{TeV}$ collected in 2011 [6] has excluded [7] the $m_{H}$ regions $112.9-115.5 \mathrm{GeV}, 131-238 \mathrm{GeV}$ and $251-466 \mathrm{GeV}$ at the $95 \% \mathrm{CL}$. The CMS results [8] based to up to $4.8 \mathrm{fb}^{-1}$ of data have excluded at the $95 \% \mathrm{CL}$ the $m_{H}$ range $127-600 \mathrm{GeV}$ [9].

The search for the SM Higgs boson through the decay $H \rightarrow Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{\prime}+\ell^{\prime}-$, where $\ell, \ell^{\prime}=e$ or $\mu$, provides good sensitivity over a wide mass range. The largest background to this search comes from continuum $\left(Z^{* *} / \gamma^{*}\right)\left(Z^{*} / \gamma^{*}\right)$ production, referred to as $Z Z^{(*)}$ hereafter. For low masses, there are also important background contributions from $Z+$ jets and $t \bar{t}$ production, where the additional charged lepton candidates arise either from decays of hadrons with $b$ - or $c$-quark content or from mis-identification of jets. Previous results from ATLAS in this channel [6] excluded the mass regions $134-156 \mathrm{GeV}$, $182-233 \mathrm{GeV}, 256-265 \mathrm{GeV}$ and $268-415 \mathrm{GeV}$ at $95 \% \mathrm{CL}$ with $4.8 \mathrm{fb}^{-1}$ of $\sqrt{s}=7 \mathrm{TeV}$ data. The corresponding search from CMS [8] excluded at $95 \%$ CL the mass regions $134-158 \mathrm{GeV}, 180-305 \mathrm{GeV}$ and $340-465 \mathrm{GeV}$.

This note updates the results presented in Ref. [6], with a new analysis of the $\sqrt{s}=7 \mathrm{TeV}$ data corresponding to an integrated luminosity of $4.8 \mathrm{fb}^{-1}$ collected in 2011, combined with the first analysis of $\sqrt{s}=8 \mathrm{TeV}$ data corresponding to an integrated luminosity of $5.8 \mathrm{fb}^{-1}$ collected between April and June 2012 [10, 11]. The analysis selection has been optimised with respect to the one described in Ref. [6] to enhance the sensitivity to a low mass Higgs boson. The $\sqrt{s}=8 \mathrm{TeV}$ data analysis benefits from substantial improvements in the electron reconstruction and identification compared to the one used for the $\sqrt{s}=7 \mathrm{TeV}$ data, which have not yet been reprocessed to take advantage of these improvements.

In the following, the ATLAS detector is briefly described in Section 2, and the signal and background simulation is presented in Section 3. The analysis of the $\sqrt{s}=8 \mathrm{TeV}$ data collected between March and June 2012 is discussed in Section 4 and that of the $\sqrt{s}=7 \mathrm{TeV}$ data collected in 2011 is described in Section 5. After a description of the systematic uncertainties in Section 6, Section 7 presents the result of the combined analysis of the two datasets.

## 2 The ATLAS Detector

The ATLAS detector [12] is a multi-purpose particle physics detector with approximately forwardbackward symmetric cylindrical geometry ${ }^{1}$. The inner tracking detector (ID) [13] covers $|\eta|<2.5$ and consists of a silicon pixel detector, a silicon micro-strip detector, and a transition radiation tracker. The ID is surrounded by a thin superconducting solenoid providing a 2 T axial magnetic field. A highgranularity lead/liquid-argon (LAr) sampling calorimeter [14] measures the energy and the position of electromagnetic showers with $|\eta|<3.2$. LAr sampling calorimeters are also used to measure hadronic showers in the end-cap ( $1.5<|\eta|<3.2$ ) and forward ( $3.1<|\eta|<4.9$ ) regions, while an iron/scintillator tile calorimeter [15] measures hadronic showers in the central region $(|\eta|<1.7)$. The muon spectrometer (MS) [16] surrounds the calorimeters and consists of three large superconducting air-core toroid magnets,

[^69]each with eight coils, a system of precision tracking chambers $(|\eta|<2.7)$, and fast tracking chambers for triggering. A three-level trigger system [17] selects events to be recorded for offline analysis.

## 3 Signal and Background Simulation

The $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ signal is modelled using the Powheg Monte Carlo (MC) event generator $[18,19]$, which calculates separately the gluon fusion and vector-boson fusion production mechanisms with matrix elements up to next-to-leading order (NLO). The Higgs boson transverse momentum ( $p_{\mathrm{T}}$ ) spectrum in the gluon fusion process follows the calculation of Ref. [20], which includes QCD corrections up to NLO and QCD soft-gluon re-summations up to next-to-next-to-leading logarithm (NNLL). Powheg is interfaced to Pythia [21,22] for showering and hadronization, which in turn is interfaced to Рнотоs [23, 24] for quantum electrodynamics (QED) radiative corrections in the final state. Pythia is used to simulate the production of a Higgs boson in association with a $W$ or a $Z$ boson.

The Higgs boson production cross sections and decay branching ratios, as well as their uncertainties, are taken from Refs. [25,26]. The cross sections for the gluon-fusion process have been calculated to next-to-leading order (NLO) [27-29], and next-to-next-to-leading order (NNLO) [30-32] in QCD. In addition, QCD soft-gluon re-summations calculated in the next-to-next-to-leading log (NNLL) approximation are applied for the gluon-fusion process [33]. NLO electroweak (EW) radiative corrections are also applied $[34,35]$. These results are compiled in Refs. [36-38] assuming factorisation between QCD and EW corrections. The cross sections for vector-boson fusion processes are calculated with full NLO QCD and EW corrections [39-41], and approximate NNLO QCD corrections are available [42]. The cross sections for the associated $W H / Z H$ production processes are calculated at NLO [43] and at NNLO [44] in QCD, and NLO EW radiative corrections [45] are applied.

The Higgs boson decay branching ratios [46] to the different four-lepton final states is provided by Prophecy4F [47, 48], which includes the complete NLO QCD+EW corrections, interference effects between identical final-state fermions, and leading two-loop heavy Higgs boson corrections to the fourfermion width. Table 1 gives the production cross sections and branching ratios for $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$, which are used to normalise the signal MC, for several Higgs boson masses.

The QCD scale uncertainties for $m_{\mathrm{H}}=125 \mathrm{GeV}$ [25] amount to ${ }_{-8}^{+7} \%$ for the gluon-fusion process and $\pm 1 \%$ for the vector-boson fusion and associated $W H / Z H$ production processes. The uncertainty of the production cross section due to uncertainties of the parton distribution function (PDF) and $\alpha_{s}$ is $\pm 8 \%$ for gluon-initiated processes and $\pm 4 \%$ for quark-initiated processes, estimated by following the prescription in Ref. [49] and by using the PDF sets of CTEQ [50], MSTW [51] and NNPDF [52]. The PDF uncertainties are assumed to be $100 \%$ correlated among processes with identical initial states, regardless of these being signal or background [49-53].

The cross section calculations do not take into account the width of the Higgs boson, which is implemented through a relativistic Breit-Wigner line shape applied at the event-generator level. In the absence of a full calculation, the possible size of such effects is included as an extra signal normalisation systematic uncertainty for $m_{H} \geq 300 \mathrm{GeV}$, on top of the one presented in Table 1, following a parametrisation as a function of $m_{H}: 150 \% \times m_{H}^{3}[\mathrm{TeV}][26]$.

The $Z Z^{(*)}$ continuum background is modelled using Powheg [54] for quark-antiquark annihilation and gg2ZZ [55] for gluon fusion, normalised to the mcFm prediction [56]. The QCD scale uncertainty has a $\pm 5 \%$ effect on the expected $Z Z^{(*)}$ background, and the effect due to the PDF and $\alpha_{s}$ uncertainties is $\pm 4 \%( \pm 8 \%)$ for quark-initiated (gluon-initiated) processes. In addition, the shape uncertainty of the four-lepton invariant mass spectrum has been assigned as discussed in Ref. [26]. For the simulation of $\tau$ lepton decays Tauola [57,58] is used. The $Z+$ jets production is modelled using Alpgen [59] and is divided into two sources: $Z+$ light jets, which includes $Z c \bar{c}$ in the massless $c$-quark approximation and $Z b \bar{b}$ from parton showers, and $Z b \bar{b}$ using matrix element calculations that take into account the $b$-quark

Table 1: Higgs boson production cross sections for gluon fusion, vector-boson fusion and associated production with a $W$ or $Z$ boson in $p p$ collisions at $\sqrt{s}$ of 7 TeV and 8 TeV [25]. The quoted uncertainties correspond to the total theoretical systematic uncertainties. The production cross section for the associated production with a $W$ or $Z$ boson is negligibly small for $m_{H}>300 \mathrm{GeV}$. The decay branching ratio for $H \rightarrow 4 \ell$, with $\ell=e$ or $\mu$, is reported in the last column [25].

| $m_{H}$ <br> $[\mathrm{GeV}]$ | $\sigma(g g \rightarrow H)$ <br> $[\mathrm{pb}]$ | $\sigma\left(q q^{\prime} \rightarrow H q q^{\prime}\right)$ <br> $[\mathrm{pb}]$ | $\sigma(q \bar{q} \rightarrow W H)$ <br> $[\mathrm{pb}]$ | $\sigma(q \bar{q} \rightarrow Z H)$ <br> $[\mathrm{pb}]$ | $\mathrm{BR}\left(H \rightarrow Z^{(*)} \rightarrow 4 \ell\right)$ <br> $\left[10^{-3}\right]$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | $\sqrt{s}=7 \mathrm{TeV}$ |  |  |
| 125 | $15.3_{-2.3}^{+3.0}$ | $1.21 \pm 0.03$ | $0.57_{-0.03}^{+0.02}$ | $0.32 \pm 0.02$ | 0.13 |
| 130 | $14.1_{-2.1}^{+2.7}$ | $1.15 \pm 0.03$ | $0.50 \pm 0.02$ | $0.28 \pm 0.01$ | 0.19 |
| 190 | $5.9_{-0.9}^{+1.0}$ | $0.69 \pm 0.02$ | $0.125 \pm 0.005$ | $0.074 \pm 0.004$ | 0.94 |
| 400 | $2.03_{-0.33}^{+0.32}$ | $0.162_{-0.005}^{+0.009}$ | - | - | 1.21 |
| 600 | $0.37 \pm 0.06$ | $0.058_{-0.002}^{+0.005}$ | - | - | 1.23 |
|  |  | $\sqrt{s}=8 \mathrm{TeV}$ |  |  |  |
| 125 | $19.5 \pm 2.9$ | $1.56_{-0.05}^{+0.04}$ | $0.70 \pm 0.03$ | $0.39 \pm 0.02$ | 0.13 |
| 130 | $18.1 \pm 2.6$ | $1.49 \pm 0.04$ | $0.61 \pm 0.03$ | $0.35 \pm 0.02$ | 0.19 |
| 190 | $7.9 \pm 1.1$ | $0.91_{-0.02}^{+0.03}$ | $0.156 \pm 0.007$ | $0.094 \pm 0.006$ | 0.94 |
| 400 | $2.9 \pm 0.4$ | $0.25 \pm 0.01$ | - | - | 1.21 |
| 600 | $0.5 \pm 0.1$ | $0.097 \pm 0.004$ | - | - | 1.23 |

mass. The MLM [60] matching scheme is used to remove any double counting of identical jets produced via the matrix element calculation and the parton shower, but this scheme is not implemented for $b$-jets. Therefore, $b \bar{b}$ pairs with separation $\Delta R=\sqrt{(\Delta \phi)^{2}+(\Delta \eta)^{2}}>0.4$ between the $b$-quarks are taken from the matrix-element calculation, whereas for $\Delta R<0.4$ the parton-shower $b \bar{b}$ pairs are used. In this search the $Z+$ jets background is normalised using control samples from data. For comparison between data and simulation, the QCD NNLO FEWz [61,62] and MCFM cross section calculations are used for inclusive $Z$ boson and $Z b \bar{b}$ production, respectively. The $t \bar{t}$ background is modelled using MC@NLO [63] and is normalised to the approximate NNLO cross section calculated using hatноr [64]. The effect of the QCD scale uncertainty of the cross section is ${ }_{-9}^{+4} \%$, while the effect of PDF and $\alpha_{s}$ uncertainties is $\pm 7 \%$. Both Alpgen and MC@NLO are interfaced to Herwig [65] for parton shower hadronization and to Jimmy [66] for the underlying event simulation.

Generated events are fully simulated using the ATLAS detector simulation [67] within the Geant4 framework [68]. Additional pp interactions in the same and nearby bunch crossings (pile-up) are included in the simulation. The MC samples are re-weighted to reproduce the observed distribution of the mean number of interactions per bunch crossing in the data.

## 4 Analysis of $\sqrt{s}=8 \mathrm{TeV}$ data

The data are subjected to quality requirements: events recorded during periods when the relevant detector components were not operating normally are rejected. The resulting integrated luminosity is $5.8 \mathrm{fb}^{-1}$.

### 4.1 Lepton Reconstruction/Identification and Event Selection

The data considered in this analysis are selected using single-lepton or di-lepton triggers. For the singlemuon trigger the transverse momentum $p_{\mathrm{T}}$ threshold is 24 GeV , while for the single-electron trigger the transverse energy, $E_{\mathrm{T}}$, threshold is 24 GeV . For the di-muon triggers the thresholds are $p_{\mathrm{T}}=13 \mathrm{GeV}$
for each muon or $p_{\mathrm{T} 1}=18 \mathrm{GeV}, p_{\mathrm{T} 2}=8 \mathrm{GeV}$ in the case of the asymmetric di-muon trigger, while for the di-electron triggers the thresholds are $E_{\mathrm{T}}=12 \mathrm{GeV}$ for each electron.

Electron candidates consist of clusters of energy deposited in the electromagnetic calorimeter that are associated to ID tracks. For the 2012 LHC data taking, the electron reconstruction algorithm has been improved with respect to 2011 , improving the performance at low $p_{\mathrm{T}}$. The ATLAS track pattern recognition and fit procedure were updated to account for energy losses due to bremsstrahlung, and the track-to-cluster matching algorithm was improved to be less sensitive to bremsstrahlung losses. Furthermore, all tracks associated to electromagnetic clusters are re-fitted using a Gaussian-Sum Filter [69], which allows for bremsstrahlung energy losses.

Electron candidates must have a well-reconstructed ID track pointing to the corresponding cluster, and the cluster should satisfy a set of identification criteria [70] that requires the longitudinal and transverse shower profiles to be consistent with those expected for electromagnetic showers. These identification criteria were optimised to maintain good performance in high pile-up conditions, and to take advantage of the new electron reconstruction. The electron transverse momentum is computed from the cluster energy and the track direction at the interaction point.

Muon candidates are formed by matching reconstructed ID tracks with either complete or partial tracks reconstructed in the MS [71]. If a complete track is present, the two independent momentum measurements are combined; otherwise the momentum is measured using the ID or the MS information alone. The muon reconstruction/identification coverage is extended by using tracks reconstructed in the forward region $(2.5<|\eta|<2.7)$ of the MS, which is outside the ID coverage. In the centre of the barrel region $(|\eta|<0.1)$, which lacks MS geometrical coverage, ID tracks with $p_{\mathrm{T}}>15 \mathrm{GeV}$ are identified as muons using the profile of the associated energy deposits in the calorimeter.

This analysis searches for Higgs boson candidates by selecting two same-flavour, opposite-sign lepton pairs in an event. The impact parameter of the leptons along the beam axis is required to be within 10 mm of the reconstructed primary vertex. To reject cosmic rays, muon tracks are required to have a transverse impact parameter, defined as the impact parameter in the bending plane with respect to the primary vertex, of less than 1 mm . The primary vertex is defined as the reconstructed vertex with the highest $\sum p_{\mathrm{T}}^{2}$ of associated tracks among the reconstructed vertices with at least three associated tracks.

Each electron (muon) must satisfy $p_{\mathrm{T}}>7 \mathrm{GeV}\left(p_{\mathrm{T}}>6 \mathrm{GeV}\right)$ and be measured in the pseudo-rapidity range $|\eta|<2.47(|\eta|<2.7)$. The most energetic lepton in the quadruplet must satisfy $p_{\mathrm{T}}>20 \mathrm{GeV}$, and the second (third) lepton in $p_{\mathrm{T}}$ order must satisfy $p_{\mathrm{T}}>15 \mathrm{GeV}\left(p_{\mathrm{T}}>10 \mathrm{GeV}\right)$. The leptons are required to be separated from each other by $\Delta R>0.1$ if they are of the same flavour and $\Delta R>0.2$ otherwise. The same-flavour and opposite-sign lepton pair closest to the $Z$ boson mass $\left(m_{Z}\right)$ is the leading di-lepton, its invariant mass, denoted by $m_{12}$, is required to be between 50 and 106 GeV . The remaining sameflavour, opposite-sign lepton pair is the sub-leading di-lepton and its invariant mass, $m_{34}$, is required to be in the range $m_{\min }<m_{34}<115 \mathrm{GeV}$, where the value of $m_{\min }$ depends on the reconstructed fourlepton invariant mass, $m_{4 \ell}$, and is shown in Table 2. All possible same-flavour opposite-charge di-lepton combinations in the quadruplet must satisfy $m_{\ell \ell}>5 \mathrm{GeV}$. Four different analysis sub-channels ( $4 e$, $2 e 2 \mu, 2 \mu 2 e, 4 \mu)$ ordered by the flavour of the leading di-lepton are defined. Data quality requirements result in slightly different integrated luminosities, $5.8 \mathrm{fb}^{-1}, 5.8 \mathrm{fb}^{-1}$ and $5.9 \mathrm{fb}^{-1}$ for the $4 \mu, 2 e 2 \mu / 2 \mu 2 e$ and $4 e$ sub-channels, respectively.

Table 2: The lower thresholds applied to $m_{34}$ for reference values of $m_{4 \ell}$. For $m_{4 \ell}$ values between these reference values the selection requirement is obtained via linear interpolation.

| $m_{4 \ell}[\mathrm{GeV}]$ | $\leq 120$ | 130 | 150 | 160 | 165 | 180 | $\geq 190$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $m_{\text {min }}$ threshold $[\mathrm{GeV}]$ | 17.5 | 22.5 | 30 | 30 | 35 | 40 | 50 |

The $Z+$ jets and $t \bar{t}$ background contributions are further reduced by applying impact parameter as well as track- and calorimeter-based isolation requirements on the leptons. The normalised track isolation discriminant is defined as the sum of the transverse momenta of tracks, $\Sigma p_{\mathrm{T}}$, inside a cone of $\Delta R<0.2$ around the lepton, excluding the lepton track, divided by the lepton $p_{\mathrm{T}}$. The tracks considered in the sum are of good quality; i.e., they have at least four hits in the pixel and silicon strip detectors ("silicon hits") and $p_{\mathrm{T}}>1 \mathrm{GeV}$ for muons, and at least nine silicon hits, one hit in the innermost pixel layer (the $b$-layer) and $p_{\mathrm{T}}>0.4 \mathrm{GeV}$ for electrons. Each lepton is required to have a normalised track isolation smaller than 0.15 .

The normalised calorimetric isolation for electrons is computed as the sum of the positive-energy topological clusters with a reconstructed barycenter falling in a cone of $\Delta R<0.2$ around the candidate electron cluster divided by the electron $p_{\mathrm{T}}$. The cut value is 0.20 . The cells within $0.125 \times 0.175$ in $\eta \times \phi$ around the electron barycenter are excluded. The algorithm for topological clusters suppresses noise by keeping only those cells with a significant energy deposit and their neighbouring cells. The ambient energy deposition in the event from pileup as well as from the underlying event is corrected for by calculating the transverse energy density from low $-p_{\mathrm{T}}$ jets, averaged over azimuth in two $\eta$ regions, and subtracting it from the isolation cone transverse energy. In the case of muons, the normalised calorimetric isolation discriminant is defined as the sum of the calorimeter cells, $\Sigma E_{T}$, inside a cone of $\Delta R<0.2$ around the muon direction, divided by the muon $p_{\mathrm{T}}$. Muons are required to have a normalised calorimetric isolation less than 0.30 ( 0.15 in case of muons without an ID track). For both the track- and calorimeter-based isolation any contributions arising from other leptons of the quadruplet are subtracted. The impact parameter significance, defined as the impact parameter divided by its uncertainty, $d_{0} / \sigma_{d_{0}}$, for all muons (electrons) is required to be lower than 3.5 (6.5). The electron impact parameter is affected by bremsstrahlung and it thus has a broader distribution.

The combined signal reconstruction and selection efficiency for $m_{H}=130 \mathrm{GeV}\left(m_{H}=360 \mathrm{GeV}\right)$ is $41 \%$ ( $67 \%$ ) for the $4 \mu$ channel, $27 \%(59 \%)$ for the $2 e 2 \mu / 2 \mu 2 e$ channel and $23 \% ~(51 \%)$ for the $4 e$ channel. The final discriminating variable for this search is $m_{4 \ell}$. The invariant mass resolution is further improved by applying a $Z$-mass constraint to the leading di-lepton for $m_{4 \ell}<190 \mathrm{GeV}$ and to both di-leptons for higher masses. The $Z$ line-shape and the experimental uncertainty in the di-lepton mass are accounted for in the $Z$-mass constraint. Figure 1 presents the $m_{4 \ell}$ distributions before and after the $Z$ mass constraint, for a simulated signal sample with $m_{H}=130 \mathrm{GeV}$, at $\sqrt{s}=8 \mathrm{TeV}$. The width of the reconstructed Higgs boson mass distribution is dominated by the experimental resolution for $m_{H}<350 \mathrm{GeV}$, while for higher $m_{H}$ the reconstructed width is dominated by the natural width of the Higgs boson. The predicted natural width of the Higgs boson is approximately 29 GeV at $m_{H}=400 \mathrm{GeV}$.

### 4.2 Background Estimation

The expected background yield and its composition is estimated using MC simulation normalised to the theoretical cross section for $Z Z^{(*)}$ production and by data-driven methods for the $\ell \ell+$ jets and $t \bar{t}$ processes. The background composition depends on the flavour of the sub-leading di-lepton and different approaches are taken for the $\ell \ell+\mu \mu$ and the $\ell \ell+e e$ final states.

### 4.2.1 $\quad \ell \ell+\mu \mu$ background

The number of $t \bar{t}$ and $Z+$ jets (dominated by $Z b \bar{b}$ ) background events in the signal region is estimated using a control region with an enhanced $b \bar{b}$ contribution. The control region is obtained by modifying the event selection as follows: no isolation requirement is applied to leptons in the sub-leading pair, and at least one of the sub-leading leptons is required to fail the impact parameter significance requirement. These modifications remove $Z Z^{(*)}$ contributions, and allow both the $t \bar{t}$ and $Z+$ jets backgrounds to be estimated simultaneously.


Figure 1: Invariant mass distributions for simulated (a) $H \rightarrow Z Z^{(*)} \rightarrow 4 \mu$, (b) $H \rightarrow Z Z^{(*)} \rightarrow 2 e 2 \mu$ and (c) $H \rightarrow Z Z^{(*)} \rightarrow 4 e$ events for $m_{H}=130 \mathrm{GeV}$, at $\sqrt{s}=8 \mathrm{TeV}$. The fitted range for the Gaussian is chosen to be: $-2 \sigma$ to $2 \sigma(-1.5 \sigma$ to $2.5 \sigma)$ for the $4 \mu(2 e 2 \mu / 4 e)$ channel. The slightly reduced mean values arise from radiative losses which are more explicit in channels involving electrons [70]. In (d), (e) and (f) the corresponding results after applying the $Z$ mass constraint are shown.

As shown in Fig. 2, the $m_{12}$ distribution is fitted using a second order Chebychev polynomial for the $t \bar{t}$ component and a Breit-Wigner line-shape convolved with a Crystal-Ball resolution function for the $Z+$ jets component. The shapes used in the fit are obtained from MC. The number of events in the control region is then extrapolated to the signal region using a transfer factor obtained from MC. The MC description of the selection efficiency has been verified with data using a control region obtained by requiring a $Z$ and exactly one extra muon. This $Z$ is selected using the leading di-lepton requirements of this analysis for the two highest $p_{\mathrm{T}}$ same-flavor opposite sign leptons. The systematic errors associated to the extrapolation from the control region to the signal region are comparable with the statistical errors of the fit.

The $t \bar{t}$ background is cross-checked using a control region defined by selecting events with an $e^{ \pm} \mu^{\mp}$ di-lepton pair with an invariant mass between 50 and 106 GeV , accompanied by an opposite sign dimuon. Events with a $Z$ candidate decaying to a pair of electrons or muons, in the aforementioned mass range, are excluded. Isolation and impact parameter requirements are applied only to the leptons of the $e \mu$ pair. In data, $16 e^{ \pm} \mu^{\mp}+\mu^{+} \mu^{-}$events are observed, to be compared with $18.9 \pm 1.1$ expected from MC.

The expected $\ell \ell+\mu \mu$ background yields in the signal region are summarised in Table 4.


Figure 2: Distribution of $m_{12}$, for $\sqrt{s}=8 \mathrm{TeV}$, in the control region where the isolation requirements are not applied to the two sub-leading muons, and at least one of these muons fails the impact parameter significance requirement. The fit used to obtain the yields for $t \bar{t}$ and $Z+$ jets is presented, the MC expectations are also shown for comparison.

### 4.2.2 $\ell \ell+e e$ background

A sample of reconstruction-level objects identified as electron candidates will contain true isolated electrons, electrons from heavy flavour semi-leptonic decays (Q), electrons from photon conversion $(\gamma)$ or light jets mis-reconstructed as electrons and denoted as fake electrons (f).

An $\ell \ell+e e$ background control region is formed by relaxing the electron selection criteria for the electrons of the sub-leading pair. The different sources of electron background are then separated into reconstruction categories which are electron-like (E), conversion-like (C) and fake-like (F), using appropriate discriminating variables [72]. The variables used are: the number of $b$-layer hits ( $n$ hits blay , the fraction of high threshold hits in the Transition Radiation Tracker ( $\mathrm{TRT}_{\text {Ratio }}$ ), the energy in the first layer of the electromagnetic calorimeter $\left(f_{1}\right)$ and the lateral containment of the cluster along $\phi$ in the second layer of the electromagnetic calorimeter $\left(R_{\phi}\right)$. The variable $n_{\text {hits }}^{\text {blayer }}$ is used to identify converted photons, and the latter three variables are used to discriminate electrons from hadrons. The numbers of observed events in each category of the control region are presented in Table 3. The expected numbers of events from MC are also given for comparison. Since only events from this control region can enter the signal region, this method directly accounts for most of the fluctuations in data. The efficiency needed to extrapolate the background yield of each category from the control region to the signal region is obtained from MC. This method estimates the sum of $Z+$ jets and $t \bar{t}$ background contributions. As a cross-check the same method is also applied to a similar control region containing same-sign sub-leading di-electrons.

The $\ell \ell+e e$ background is also estimated using a control region with same-sign sub-leading dielectrons, where the three highest $p_{\mathrm{T}}$ leptons satisfy all the analysis criteria and the remaining electron is required to only fulfill the good track criteria (silicon hits $>=7$ and pixel hits $>=1$ ) and the lateral containment of the cluster energy along $\eta\left(R_{\eta}\right)$. This method will be referred to as $3 \ell+\ell$ hereafter. In this case a simultaneous fit of templates, obtained from the $n_{\text {hits }}^{\text {blayer }}$ and the $\mathrm{TRT}_{\text {Ratio }}$ distributions, is used to estimate the yields for the different truth components: $\mathrm{f}, \gamma$ and Q . The templates used are obtained from MC. The fits for the $2 \mu 2 e$ and $4 e$ sub-channels are presented in Fig. 3. Additional checks are performed

Table 3: The observed yields of the various categories in the $\ell \ell+e e$ control region for $\sqrt{s}=8 \mathrm{TeV}$. Events are classified according to whether the electron candidates of the sub-leading di-electrons are: electron-like (E), conversion-like (C) and fake-like (F). For comparison the MC expectations are also shown. The di-lepton categorisation in reconstruction categories is ordered in $p_{\mathrm{T}}$.

|  | $4 e$ |  | $2 \mu 2 e$ |  |
| :--- | :---: | ---: | :---: | ---: |
|  | Data | MC | Data | MC |
| EE | 32 | $22.7 \pm 4.8$ | 31 | $24.9 \pm 5.0$ |
| EC | 6 | $6.0 \pm 2.5$ | 2 | $1.9 \pm 1.4$ |
| EF | 18 | $19.0 \pm 4.4$ | 26 | $15.3 \pm 3.9$ |
| CE | 4 | $8.8 \pm 3.0$ | 6 | $5.1 \pm 2.3$ |
| CC | 1 | $5.3 \pm 2.3$ | 6 | $4.2 \pm 2.0$ |
| CF | 12 | $8.8 \pm 3.0$ | 15 | $15.3 \pm 3.9$ |
| FE | 16 | $5.7 \pm 2.4$ | 12 | $8.4 \pm 2.9$ |
| FC | 6 | $6.5 \pm 2.6$ | 7 | $4.3 \pm 2.1$ |
| FF | 12 | $17.4 \pm 4.2$ | 16 | $33.6 \pm 5.8$ |
| Total | 107 | $100 \pm 10$ | 121 | $113 \pm 11$ |

by replacing the $\operatorname{TRT}_{\text {Ratio }}$ with $f_{1}$ or the distance in $\eta$ between the extrapolated impact point of the track on the calorimeter and the cluster barycenter using the strips $\left(\Delta \eta_{1}\right)$. The difference in the results is taken into account as a systematic error.

Finally, the $\ell \ell+e e$ background is also estimated by performing the full analysis but selecting samesign pairs for the sub-leading di-electrons. In this case, there remain 4 (3) events below $m_{4 \ell}=160 \mathrm{GeV}$ in the $4 e(2 \mu 2 e)$ sub-channel.

The expected $\ell \ell+e e$ background yields in the signal region are summarised in Table 4.

### 4.2.3 Summary of background estimates

The results of all the background estimation methods are summarised in Table 4. The $m_{12}$ and $m_{34}$ distributions, for events selected by the analysis when relaxing the isolation and impact parameter requirements for the sub-leading di-lepton, are presented in Fig. 4. The events are divided according to the flavour of the sub-leading lepton pair into $\ell \ell+\mu \mu$ and $\ell \ell+e e$ samples. In Figs. 4(a) and 4(c) the $m_{12}$ and $m_{34}$ distributions are presented for $\ell \ell+\mu \mu$ events, while in Figs. 4(b) and 4(d) the corresponding distributions are presented for $\ell \ell+e e$ events. The shape and normalisation of the backgrounds discussed earlier are in good agreement with data. This is observed both for large values of $m_{34}$, where the $Z Z^{(*)}$ background dominates, and for low $m_{34}$ values.


Figure 3: The results of a simultaneous fit to (a) $n_{\text {hits }}^{\text {blayer }}$ and (b) $\mathrm{TRT}_{\text {Ratio }}$ for the background components in the $2 \mu 2 e$ channel. In (c) and (d) the corresponding results for the $4 e$ channel are given. The sources of background electrons are denoted as: light jets faking an electron ( f ), photon conversions ( $\gamma$ ) and electrons from heavy quark semi-leptonic decays ( Q ).

Table 4: Summary of the background estimates for the $\sqrt{s}=8 \mathrm{TeV}$ data. The " $\dagger$ " symbol indicates the estimated number of events used for the background normalisation, the others being cross-checks. The first uncertainty is statistical, while the second is systematic.

| Method | Estimated <br> number of events |  |
| :---: | :---: | :---: |
| $4 \mu$ |  |  |
| $m_{12}$ fit: $Z+$ jets contribution | $0.51 \pm 0.13 \pm 0.16^{\dagger}$ |  |
| $m_{12}$ fit: $t \bar{t}$ contribution | $0.044 \pm 0.015 \pm 0.015^{\dagger}$ |  |
| $t \bar{t}$ from $e^{ \pm} \mu^{\mp}+\mu^{ \pm} \mu^{\mp}$ | $0.058 \pm 0.015 \pm 0.019$ |  |
| $2 e 2 \mu$ |  |  |
| $m_{12}$ fit: $Z+$ jets contribution | $0.41 \pm 0.10 \pm 0.13^{\dagger}$ |  |
| $m_{12}$ fit: $t \bar{t}$ contribution | $0.040 \pm 0.013 \pm 0.013^{\dagger}$ |  |
| $t \bar{t}$ from $e^{ \pm} \mu^{\mp}+\mu^{ \pm} \mu^{\mp}$ | $0.051 \pm 0.013 \pm 0.017$ |  |
| $2 \mu 2 e$ |  |  |
| $\ell \ell+e^{ \pm} e^{\mp}$ | $4.9 \pm 0.8 \pm 0.7^{\dagger}$ |  |
| $\ell \ell e^{ \pm} e^{ \pm}$ | $4.1 \pm 0.6 \pm 0.8$ |  |
| $3 \ell+\ell$ (same-sign) | $3.5 \pm 0.5 \pm 0.5$ |  |
| $\ell \ell+e^{ \pm} e^{\mp}$ | $4 e$ |  |
| $\ell \ell+e^{ \pm} e^{ \pm}$ | $3.9 \pm 0.7 \pm 0.8^{\dagger}$ |  |
| $3 \ell+\ell$ (same-sign) | $3.1 \pm 0.5 \pm 0.6$ |  |
|  | $3.0 \pm 0.4 \pm 0.4$ |  |



Figure 4: Invariant mass distributions of the lepton pairs in the control sample defined by a $Z$ boson candidate and an additional same-flavour lepton pair, for the $\sqrt{s}=8 \mathrm{TeV}$ dataset. The sample is divided according to the flavour of the additional lepton pair. In (a) the $m_{12}$ and in (c) the $m_{34}$ distributions are presented for $\ell \ell\left(\mu^{+} \mu^{-} / e^{+} e^{-}\right)+\mu^{+} \mu^{-}$events. In (b) the $m_{12}$ and in (d) the $m_{34}$ distributions are presented for $\ell \ell\left(\mu^{+} \mu^{-} / e^{+} e^{-}\right)+e^{+} e^{-}$events. The kinematic selection of the analysis is applied. Isolation and impact parameter significance requirements are applied to the first lepton pair only. The MC is normalized to the data driven background estimations given in Table 4.

## 5 Analysis of $\sqrt{s}=7 \mathrm{TeV}$ data

In this section the analysis of the $2011 \sqrt{s}=7 \mathrm{TeV}$ data, using the same kinematic selection as the $\sqrt{s}=8 \mathrm{TeV}$ analysis, is presented.

The data collected during 2011 are subjected to quality requirements similar to those used for the 2012 data. The resulting integrated luminosity being $4.8 \mathrm{fb}^{-1}, 4.8 \mathrm{fb}^{-1}$ and $4.9 \mathrm{fb}^{-1}$ for the $4 \mu, 2 e 2 \mu / 2 \mu 2 e$ and $4 e$ final states, respectively.

### 5.1 Lepton Reconstruction/Identification and Event Selection

The data considered in this analysis are selected using single-lepton or di-lepton triggers. For the singlemuon trigger the $p_{\mathrm{T}}$ threshold is 18 GeV , while for the single-electron trigger the $E_{\mathrm{T}}$ threshold is $20-22 \mathrm{GeV}$ depending on the LHC data-taking period. For the di-muon and di-electron triggers the thresholds are $p_{\mathrm{T}}=10 \mathrm{GeV}$ for each muon, and $E_{\mathrm{T}}=12 \mathrm{GeV}$ for both electrons.

For the $\sqrt{s}=7 \mathrm{TeV}$ dataset, the electron reconstruction proceeds as described in Ref. [70], with the exception that electron candidates are refitted using a Gaussian-sum filter [73], which recovers electron candidates that suffered large energy losses due to bremsstrahlung emissions. Electron reconstruction and identification is similar to that used in Ref. [6].

The event selection is identical between $\sqrt{s}=7 \mathrm{TeV}$ and 8 TeV data analyses with the following exceptions:

- For the electron track isolation, tracks are required to have at least seven silicon hits, one $b$-layer hit and $p_{\mathrm{T}}>1 \mathrm{GeV}$.
- The calorimeter isolation of electrons in 2011 is cell-based rather than topological cluster based and the actual cut is 0.3 instead of 0.2 .

The combined signal reconstruction and selection efficiency for $m_{H}=130 \mathrm{GeV}\left(m_{H}=360 \mathrm{GeV}\right)$ is $43 \%$ ( $70 \%$ ) for the $4 \mu$ channel, $23 \%(56 \%)$ for the $2 e 2 \mu / 2 \mu 2 e$ channel and $17 \% ~(45 \%)$ for the $4 e$ channel.

### 5.2 Background Estimation

The background estimation strategy in the $\sqrt{s}=7 \mathrm{TeV}$ data sample is identical to the $\sqrt{s}=8 \mathrm{TeV}$ one, described in Section 4.2.

The estimation of the $t \bar{t}$ and $Z+$ jets (dominated by $Z b \bar{b}$ ) background events in the signal region using the fit in $m_{12}$, described in Section 4.2.1, is shown in Fig. 5. For the $e^{ \pm} \mu^{\mp}+\mu^{+} \mu^{-}$control region 8 events are observed in data with $11.0 \pm 0.6$ expected from MC. For the $\ell \ell+e e$ control region (defined in Section 4.2.2), the number of events observed in the dataset from $\sqrt{s}=7 \mathrm{TeV}$ in each category of the control region are summarised in Table 5. The final expectations in the signal region are summarised in Table 6.

The $\ell \ell+e e$ background estimate from performing the full analysis but selecting same-sign pairs for the sub-leading di-electrons gives 4 (1) events below $m_{4 \ell}=160 \mathrm{GeV}$ in the $4 e(2 \mu 2 e)$ sub-channel.

Figure 6 displays the invariant masses of lepton pairs in events with a $Z$ boson candidate and an additional same-flavour lepton pair, selected by applying the kinematic requirements of the analysis, and by applying isolation requirements to the first lepton pair only. The events are divided according to the flavour of the additional lepton pair into $\ell \ell+\mu \mu$ and $\ell \ell+e e$ samples. In Figs. 6(a) and 6(c) the $m_{12}$ and $m_{34}$ distributions are presented for $\ell \ell+\mu \mu$ events, while in Figs. 6(b) and 6(d) the corresponding distributions are presented for $\ell \ell+e e$ events. The shape and normalisation of the backgrounds discussed earlier are in good agreement with data; this is observed both for large values of $m_{34}$, where the $Z Z^{(*)}$ background dominates, and for low $m_{34}$ values.


Figure 5: Distribution of $m_{12}$, for $\sqrt{s}=7 \mathrm{TeV}$, in the control region where the isolation requirements are not applied to the two sub-leading muons, and at least one of these muons fails the impact parameter significance requirement. The fit used to obtain the yields for $t \bar{t}$ and $Z+$ jets is presented, the MC expectations are also shown for comparison.

Table 5: The observed yields of the various categories in the $\ell \ell+e e$ control region for $\sqrt{s}=7 \mathrm{TeV}$. Events are classified according to whether the electron candidates of the sub-leading di-electrons are: electron-like (E), conversion-like (C) and fake-like (F). For comparison the MC expectations are also shown. The di-lepton categorization in reconstruction categories is ordered in $p_{\mathrm{T}}$.

|  | $4 e$ |  | $2 \mu 2 e$ |  |
| :--- | :---: | :---: | :---: | :---: |
|  | Data | MC | Data | MC |
| EE | 11 | $11.2 \pm 0.6$ | 8 | $15.0 \pm 0.9$ |
| EC | 4 | $2.5 \pm 0.8$ | 3 | $3.0 \pm 1.1$ |
| EF | 6 | $9.7 \pm 1.4$ | 5 | $6.6 \pm 1.1$ |
| CE | 5 | $1.5 \pm 0.7$ | 6 | $4.5 \pm 1.6$ |
| CC | 2 | $1.4 \pm 0.7$ | 2 | $1.5 \pm 1.0$ |
| CF | 7 | $4.7 \pm 1.2$ | 10 | $9.9 \pm 2.3$ |
| FE | 5 | $3.1 \pm 0.6$ | 4 | $4.5 \pm 1.0$ |
| FC | 5 | $3.0 \pm 1.0$ | 4 | $6.3 \pm 1.8$ |
| FF | 12 | $11.0 \pm 1.9$ | 17 | $13.4 \pm 2.6$ |
| Total | 57 | $48 \pm 3$ | 59 | $65 \pm 5$ |

Table 6: Summary of the background estimates for the $\sqrt{s}=7 \mathrm{TeV}$ data sample. The " $\dagger$ " symbol indicates the estimated number of events used for the background normalisation, the others being crosschecks. The first uncertainty is statistical, while the second is systematic.

| Method | Estimated <br> number of events |
| :---: | :---: |
| $4 \mu$ |  |
| $m_{12}$ fit: $Z+$ jets contribution | $0.25 \pm 0.10 \pm 0.08^{\dagger}$ |
| $m_{12}$ fit: $t \bar{t}$ contribution | $0.022 \pm 0.010 \pm 0.011^{\dagger}$ |
| $t \bar{t}$ from $e^{ \pm} \mu^{\mp}+\mu^{ \pm} \mu^{\mp}$ | $0.025 \pm 0.009 \pm 0.014$ |
| $2 e 2 \mu$ |  |
| $m_{12}$ fit: $Z+$ jets contribution | $0.20 \pm 0.08 \pm 0.06^{\dagger}$ |
| $m_{12}$ fit: $t \bar{t}$ contribution | $0.020 \pm 0.009 \pm 0.011^{\dagger}$ |
| $t \bar{t}$ from $e^{ \pm} \mu^{\mp}+\mu^{ \pm} \mu^{\mp}$ | $0.024 \pm 0.009 \pm 0.014$ |
| $2 \mu 2 e$ |  |
| $\ell \ell+e^{ \pm} e^{\mp}$ | $2.6 \pm 0.4 \pm 0.4^{\dagger}$ |
| $\ell \ell+e^{ \pm} e^{ \pm}$ | $3.7 \pm 0.9 \pm 0.6$ |
| $3 \ell+\ell($ same-sign $)$ | $2.0 \pm 0.5 \pm 0.3$ |
| $\quad 4 e$ |  |
| $\ell \ell+e^{ \pm} e^{\mp}$ | $3.1 \pm 0.6 \pm 0.5^{\dagger}$ |
| $\ell \ell+e^{ \pm} e^{ \pm}$ | $3.2 \pm 0.6 \pm 0.5$ |
| $3 \ell+\ell$ (same-sign) | $2.2 \pm 0.5 \pm 0.3$ |



Figure 6: Invariant mass distributions of the lepton pairs in the control sample defined by a $Z$ boson candidate and an additional same-flavour lepton pair for the $\sqrt{s}=7 \mathrm{TeV}$ data sample. The sample is divided according to the flavour of the additional lepton pair. In (a) the $m_{12}$ and in (c) the $m_{34}$ distributions are presented for $\ell \ell\left(\mu^{+} \mu^{-} / e^{+} e^{-}\right)+\mu^{+} \mu^{-}$events. In (b) the $m_{12}$ and in (d) the $m_{34}$ distributions are presented for $\ell \ell\left(\mu^{+} \mu^{-} / e^{+} e^{-}\right)+e^{+} e^{-}$events. The kinematic selections of the analysis are applied. Isolation requirements are applied to the first lepton pair only. The MC is normalized to the data driven background estimations given in Table 6.

## 6 Systematic Uncertainties

The uncertainty of the lepton reconstruction and identification efficiencies, and of the momentum resolution and scale, are determined using samples of $W, Z$ and $J / \psi$ decays [70]. The uncertainty of the muon identification and reconstruction efficiency results in a relative acceptance uncertainty of the signal and the $Z Z^{(*)}$ background which is uniform over the mass range of interest, and amounts to $\pm 0.16 \% ~( \pm 0.12 \%)$ for the $4 \mu(2 e 2 \mu)$ channel. The uncertainty of the electron identification efficiency results in a relative acceptance uncertainty of $\pm 3.0 \%( \pm 1.7 \%)$ for the $4 e(2 e 2 \mu)$ channel at $m_{4 \ell}=600 \mathrm{GeV}$ and reaches $\pm 8.0 \%( \pm 4.6 \%)$ at $m_{4 \ell}=110 \mathrm{GeV}$. The effects of muon momentum resolution and scale uncertainty are found to be negligible. The effect of the uncertainty of the energy resolution for electrons is negligible, while the uncertainty of the electron energy scale results in an uncertainty of less than $\pm 0.7 \%$ ( $\pm 0.4 \%$ ) on the mass scale of the $m_{4 \ell}$ distribution for the $4 e(2 e 2 \mu)$ channel.

The selection efficiency of the isolation and impact parameter requirements is studied using data for both isolated and non-isolated leptons. Isolated leptons are obtained from $Z \rightarrow \ell \ell$ decays, while additional leptons reconstructed in events with $Z \rightarrow \ell \ell$ decays constitute the sample of non-isolated leptons. Additional checks are performed with non-isolated leptons from semi-leptonic $b$ - and $c$-quark decays in a heavy-flavour enriched di-jet sample. Good agreement is observed between data and simulation and the systematic uncertainty is, in general, estimated to be small with respect to the other systematic uncertainties.

An additional uncertainty on the signal selection efficiency is added in the 2011 analysis only, which is not needed in the 2012 analysis due to an improved modelling of the signal kinematics. This additional uncertainty is evaluated by varying the Higgs boson $p_{\mathrm{T}}$ spectrum in the gluon fusion process according to the PDF and QCD scale uncertainties.

The background uncertainties of the data driven methods have already been presented in Sections 4 and 5. The overall uncertainty of the integrated luminosity for the complete 2011 dataset is $\pm 1.8 \%$ and is described in Refs. [10, 11]. For the 2012 dataset the corresponding preliminary uncertainty is $\pm 3.6 \%$ based on the calibration described in Ref. [11].

The theory-related systematic uncertainty, for both signal and $Z Z^{(*)}$ background, has been discussed in Section 3. The uncertainties related to the data-driven methods are summarised in Tables 4 and 6.

## 7 Results

In Table 7, the numbers of events observed in each final state are summarised and compared to the expected backgrounds, separately for $m_{4 \ell}<160 \mathrm{GeV}$ and $m_{4 \ell} \geq 160 \mathrm{GeV}$, and to the expected signal for various $m_{H}$ hypotheses. Table 8 presents the observed and expected events, in a window of $\pm 5 \mathrm{GeV}$ around various hypothesized Higgs boson masses, for the $5.8 \mathrm{fb}^{-1}$ at $\sqrt{s}=8 \mathrm{TeV}$ and the $4.8 \mathrm{fb}^{-1}$ at $\sqrt{s}=7 \mathrm{TeV}$ datasets as well as for their combination.

The expected $m_{4 \ell}$ distributions for the total background and several signal hypotheses are compared to the data in Fig. 7. Figure 8 presents the same distributions only for the low mass range $80-250 \mathrm{GeV}$. In Figures 9 and 10 the $m_{4 \ell}$ mass distributions for each sub-channel $(4 \mu, 2 \mu 2 e, 2 e 2 \mu, 4 e)$ are shown for the data at $\sqrt{s}=8 \mathrm{TeV}$ and $\sqrt{s}=7 \mathrm{TeV}$, respectively. High- $p_{\mathrm{T}}$ photon emissions from final-state radiation (FSR), although occurring at a low rate, are not taken into account explicitely in the lepton reconstruction, and affect the reconstructed invariant mass in rare cases. In MC, QED corrections are fully considered and accounted for in the templates used for the mass distributions. All candidates selected have been checked and no appreciable FSR activity has been found for the candidates below 160 GeV .

Upper limits are set on the Higgs boson production cross section at $95 \% \mathrm{CL}$, using the $C L_{s}$ modified frequentist formalism [74] with the profile likelihood ratio test statistic [75]. The test statistic is evaluated using a maximum-likelihood fit of signal and background models to the observed $m_{4 \ell}$ distribution.

Table 7: The observed numbers of events and the final estimate for the expected backgrounds, separated into "Low mass" ( $m_{4 \ell}<160 \mathrm{GeV}$ ) and "High mass" ( $m_{4 \ell} \geq 160 \mathrm{GeV}$ ) regions. The expected numbers of signal events is also shown for various Higgs boson mass hypotheses. For signal and background estimates, the corresponding total uncertainty is given.

|  | $4 \mu$ |  | $2 e 2 \mu / 2 \mu 2 e$ |  | $4 e$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Low mass | High mass | Low mass | High mass | Low mass | High mass |
| $\sqrt{s}=8 \mathrm{TeV}$ |  |  |  |  |  |  |
| Int. Luminosity | $5.8 \mathrm{fb}^{-1}$ |  | $5.8 \mathrm{fb}^{-1}$ |  | $5.9 \mathrm{fb}^{-1}$ |  |
| ZZ ${ }^{(*)}$ | $6.3 \pm 0.3$ | $27.5 \pm 1.9$ | $3.7 \pm 0.2$ | $41.7 \pm 3.0$ | $2.9 \pm 0.3$ | $17.7 \pm 1.4$ |
| $Z+$ jets, and $t \bar{t}$ | $0.4 \pm 0.2$ | $0.15 \pm 0.07$ | $3.9 \pm 0.9$ | $1.4 \pm 0.3$ | $2.9 \pm 0.8$ | $1.0 \pm 0.3$ |
| Total Background | $6.7 \pm 0.3$ | $27.6 \pm 1.9$ | $7.6 \pm 1.0$ | $43.1 \pm 3.0$ | $5.7 \pm 0.8$ | $18.8 \pm 1.4$ |
| Data | 4 | 34 | 11 | 61 | 7 | 25 |
| $m_{H}=125 \mathrm{GeV}$ |  |  |  |  |  |  |
| $m_{H}=150 \mathrm{GeV}$ |  |  |  |  |  |  |
| $m_{H}=190 \mathrm{GeV}$ |  |  | 12.5 | +1.7 |  | 0.8 |
| $m_{H}=400 \mathrm{GeV}$ |  | 0.5 |  |  |  | 0.4 |
| $\sqrt{s}=7 \mathrm{TeV}$ |  |  |  |  |  |  |
| Int. Luminosity | $4.8 \mathrm{fb}^{-1}$ |  | $4.8 \mathrm{fb}^{-1}$ |  | $4.9 \mathrm{fb}^{-1}$ |  |
| $Z Z^{(*)}$ | $4.9 \pm 0.2$ | $18.1 \pm 1.3$ | $3.1 \pm 0.2$ | $27.3 \pm 2.0$ | $1.6 \pm 0.2$ | $10.2 \pm 0.8$ |
| $Z+$ jets, and $t \bar{t}$ | $0.2 \pm 0.1$ | $0.07 \pm 0.03$ | $2.1 \pm 0.5$ | $0.7 \pm 0.2$ | $2.3 \pm 0.6$ | $0.8 \pm 0.2$ |
| Total Background | $5.1 \pm 0.2$ | $18.2 \pm 1.3$ | $5.1 \pm 0.5$ | $28.0 \pm 2.0$ | $3.9 \pm 0.6$ | $11.0 \pm 0.8$ |
| Data | 8 | 25 | 5 | 28 | 4 | 18 |
| $m_{H}=125 \mathrm{GeV}$ |  |  |  |  | 0.37 | 0.05 |
| $m_{H}=150 \mathrm{GeV}$ |  |  |  |  |  | 0.2 |
| $m_{H}=190 \mathrm{GeV}$ |  | 0.6 |  | 1.0 |  | 0.4 |
| $m_{H}=400 \mathrm{GeV}$ |  |  |  |  |  | 0.2 |

Table 8: The numbers of expected signal and background events together with the number of observed events, in a window of $\pm 5 \mathrm{GeV}$ around the hypothesized Higgs boson mass for the $5.8 \mathrm{fb}^{-1}$ at $\sqrt{s}=8 \mathrm{TeV}$ and the $4.8 \mathrm{fb}^{-1}$ at $\sqrt{s}=7 \mathrm{TeV}$ datasets as well as for their combination.

| $\sqrt{s}=8 \mathrm{TeV}$ |  |  |  | $\sqrt{s}=7$ |  |  | $\sqrt{s}=8 \mathrm{TeV}$ and | nd $\sqrt{s}=7$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $4 \mu$ |  |  |  |  |  |  |  |  |  |
|  | exp. signal | exp. bkg |  | exp. signal | exp. bkg |  | exp. signal | exp. bkg | obs |
| 120 | $0.68 \pm 0.09$ | $0.61 \pm 0.04$ | 2 | $0.48 \pm 0.06$ | $0.46 \pm 0.03$ | 2 | $1.16 \pm 0.15$ | $1.07 \pm 0.07$ | 4 |
| 125 | $1.25 \pm 0.17$ | $0.74 \pm 0.05$ | 4 | $0.84 \pm 0.11$ | $0.56 \pm 0.03$ | 2 | $2.09 \pm 0.28$ | $1.30 \pm 0.08$ | 6 |
| 130 | $1.88 \pm 0.25$ | $0.81 \pm 0.05$ | 2 | $1.38 \pm 0.18$ | $0.63 \pm 0.03$ | 1 | $3.26 \pm 0.43$ | $1.44 \pm 0.08$ | 3 |
| $2 e 2 \mu / 2 \mu 2 e$ |  |  |  |  |  |  |  |  |  |
|  | exp. signal | exp. bkg | obs | exp. signal | exp. bkg |  | exp. signal | exp. bkg | obs |
| 120 | $0.81 \pm 0.12$ | $1.15 \pm 0.17$ | 2 | $0.48 \pm 0.07$ | $0.78 \pm 0.10$ | 1 | $1.29 \pm 0.19$ | $1.93 \pm 0.18$ | 3 |
| 125 | $1.45 \pm 0.20$ | $1.30 \pm 0.19$ | 3 | $0.83 \pm 0.11$ | $0.89 \pm 0.11$ | 2 | $2.28 \pm 0.31$ | $2.19 \pm 0.21$ | 5 |
| 130 | $2.24 \pm 0.32$ | $1.34 \pm 0.20$ | 2 | $1.27 \pm 0.17$ | $0.94 \pm 0.11$ | 1 | $3.51 \pm 0.49$ | $2.28 \pm 0.21$ | 3 |
| $4 e$ |  |  |  |  |  |  |  |  |  |
|  | exp. signal | exp. bkg | obs | exp. signal | exp. bkg |  | exp. signal | exp. bkg | obs |
| 120 | $0.35 \pm 0.05$ | $0.79 \pm 0.15$ | 1 | $0.15 \pm 0.02$ | $0.60 \pm 0.12$ | 1 | $0.50 \pm 0.07$ | $1.39 \pm 0.19$ | 2 |
| 125 | $0.61 \pm 0.09$ | $0.90 \pm 0.17$ | 2 | $0.28 \pm 0.04$ | $0.69 \pm 0.13$ | 0 | $0.89 \pm 0.13$ | $1.59 \pm 0.22$ | 2 |
| 130 | $0.91 \pm 0.15$ | $0.96 \pm 0.17$ | 1 | $0.42 \pm 0.06$ | $0.74 \pm 0.14$ | 0 | $1.33 \pm 0.21$ | $1.70 \pm 0.22$ | 1 |



Figure 7: The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates compared to the background expectation in the range $80-600 \mathrm{GeV}$ for the (a) $\sqrt{s}=8 \mathrm{TeV} 8$ and (b) $\sqrt{s}=7 \mathrm{TeV}$ datasets. The error bars represent the $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown. The resolution of the reconstructed Higgs boson mass is dominated by detector resolution at low $m_{H}$ values and by the Higgs boson width at high $m_{H}$.

Figures 11, 12 and 13 show the observed and expected $95 \%$ CL cross section upper limits, as a function of $m_{H}$, for the $\sqrt{s}=8 \mathrm{TeV}$ data, the $\sqrt{s}=7 \mathrm{TeV}$ data and for the combination of the two datasets. Combining the two datasets, the SM Higgs boson is excluded at $95 \% \mathrm{CL}$ in the mass ranges $131-162 \mathrm{GeV}$ and $170-460 \mathrm{GeV}$. The expected exclusion ranges are $124-164 \mathrm{GeV}$ and $176-500 \mathrm{GeV}$.


Figure 8: The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates compared to the background expectation in the $80-250 \mathrm{GeV}$ mass range for the (a) $\sqrt{s}=8 \mathrm{TeV}$ and (b) $\sqrt{s}=7 \mathrm{TeV}$ datasets. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown.

The significance of an excess is given by the probability, $p_{0}$, that a background-only experiment is more signal-like in terms of the test statistic than the observed data. In Figure 14 the local $p_{0}$, obtained using the asymptotic approximation of Ref. [75], is presented as a function of the $m_{H}$ hypothesis for the combination of $\sqrt{s}=8$ and 7 TeV data samples. For comparison the results for the two data samples are given separately in Fig. 15.

The most significant upward deviations from the background-only hypothesis in the $\sqrt{s}=7 \mathrm{TeV}$ data are observed for $m_{H}=242 \mathrm{GeV}$ with a local $p_{0}$ of $0.5 \%$ ( 2.6 standard deviations), and for $m_{H}=125 \mathrm{GeV}$ with a local $p_{0}$ of $1.1 \%$ ( 2.3 standard deviations). In the $\sqrt{s}=8 \mathrm{TeV}$ data, they are at $m_{H}=125.5 \mathrm{GeV}$ with a local $p_{0}$ of $0.4 \%$ ( 2.7 standard deviations), and for $m_{H}=266 \mathrm{GeV}$ with a local $p_{0}$ of $3.5 \%$ ( 1.8 standard deviations). In the combined analysis of the two datasets, the lowest local $p_{0}$ value is $0.029 \%$ ( 3.4 standard deviations), at $m_{H}=125 \mathrm{GeV}$. The probability that such an excess occurs anywhere in the full mass range considered in this search (i.e., the look-elsewhere effect on the above $p_{0}$ value), is evaluated using the method of Ref. [76], using the mass range between 110 GeV and 141 GeV (i.e., the mass range not previously excluded at the $95 \%$ C.L. by the LHC experiments [77]). The global $p_{0}$ of the excess located at $m_{H}=125 \mathrm{GeV}$ is $0.65 \%$, or 2.5 standard deviations. In the high mass region ( $m_{H}>160 \mathrm{GeV}$ ), the lowest $p_{0}$ is at $1.9 \%$ ( 2.1 standard deviations), at $m_{H}=266 \mathrm{GeV}$.

To determine the potential effect on the $p_{0}$ due to the $S M Z Z^{(*)}$ production normalisation, a test is performed where the $Z Z^{(*)}$ normalisation is obtained directly from the data. No significant modification of the observed and expected $p_{0}$ in the low $m_{H}$ region is observed.

In Fig. 16(a) the signal strength parameter $\mu=\sigma / \sigma_{S M}$ is presented as a function of $m_{H}$ for the combination of the two data samples. The corresponding result in the case where a SM Higgs signal of $m_{H}=125 \mathrm{GeV}$ is injected is shown in Fig. 16(b). The bands illustrate the $\mu$ interval corresponding to $-2 \ln \lambda(\mu)<1$, where $\lambda$ is the profile likelihood ratio test statistic, and represent an approximate $\pm 1 \sigma$ variation. The fitted signal strength divided by the expected SM rate is denoted with $\hat{\mu}$. The expected $\hat{\mu}$ has an asymmetric shape and because the expected SM rate rises rapidly with $m_{H}$ in the low mass region, the expected $\hat{\mu}$ is increased below the injected signal mass and slightly exceeds one for a small mass


Figure 9: The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates for the $\sqrt{s}=8 \mathrm{TeV}$ analysis, for the various sub-channels (a) $4 \mu$, (b) $2 \mu 2 e$, (c) $2 e 2 \mu$, (d) $4 e$, compared to the background expectation for the $80-250 \mathrm{GeV}$ mass range. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown.
range.
Figure 17 presents the best $\mu$ and $m_{H}$ fit and the profile likelihood ratio contours that, in the asymptotic limit, would correspond to $68 \%$ and $95 \%$ confidence levels.

## 8 Summary

A search for the SM Higgs boson in the decay channel $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ based on $4.8 \mathrm{fb}^{-1}$ of data recorded with the ATLAS detector at $\sqrt{s}=7 \mathrm{TeV}$ during 2011 and $5.8 \mathrm{fb}^{-1}$ recorded at $\sqrt{s}=8 \mathrm{TeV}$ during 2012 has been presented. The SM Higgs boson is excluded at $95 \%$ CL in the mass ranges $131-$ 162 GeV and $170-460 \mathrm{GeV}$. An excess of events is observed around $m_{H}=125 \mathrm{GeV}$, whose $p_{0}$ value is


Figure 10: The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates for the $\sqrt{s}=7 \mathrm{TeV}$ analysis for the various sub-channels (a) $4 \mu$, (b) $2 \mu 2 e$, (c) $2 e 2 \mu$, (d) $4 e$, compared to the background expectation for the $80-250 \mathrm{GeV}$ mass range. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown.
$0.029 \%$ ( 3.4 standard deviations) in the combined analysis of the two datasets.


Figure 11: The expected (dashed) and observed (full line) 95\% CL upper limits on the Standard Model Higgs boson production cross section as a function of $m_{H}$, divided by the expected SM Higgs boson cross section, for the $\sqrt{s}=8 \mathrm{TeV}$ data sample. The dark (green) and light (yellow) bands indicate the expected limits with $\pm 1 \sigma$ and $\pm 2 \sigma$ fluctuations, respectively; (a) shows the low mass range, and (b) the full range under consideration.


Figure 12: The expected (dashed) and observed (full line) 95\% CL upper limits on the SM Higgs boson production cross section as a function of $m_{H}$, divided by the expected SM Higgs boson cross section for the $\sqrt{s}=7 \mathrm{TeV}$ data sample. The dark (green) and light (yellow) bands indicate the expected limits with $\pm 1 \sigma$ and $\pm 2 \sigma$ fluctuations, respectively; (a) shows the low mass range, and (b) the full range under consideration.


Figure 13: The expected (dashed) and observed (full line) $95 \%$ CL upper limits on the Standard Model Higgs boson production cross section as a function of $m_{H}$, divided by the expected SM Higgs boson cross section, for the combination of the $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data samples. The dark (green) and light (yellow) bands indicate the expected limits with $\pm 1 \sigma$ and $\pm 2 \sigma$ fluctuations, respectively; (a) shows the low mass range, and (b) the full range under consideration.


Figure 14: The observed local $p_{0}$ for the combination of the 2011 and 2012 datasets (solid line). The dashed curve shows the expected median local $p_{0}$ for the signal hypothesis when tested at the corresponding $m_{H}$. The horizontal dashed lines indicate the $p_{0}$ values corresponding to local significances of $1 \sigma, 2 \sigma, 3 \sigma$ and $4 \sigma$.


Figure 15: The observed local $p_{0}$ for the combination of the 2011 and 2012 datasets (solid black line); the $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data results are shown in solid lines (blue and red, respectively). The dashed curves show the expected median local $p_{0}$ for the signal hypothesis when tested at the corresponding $m_{H}$. The horizontal dashed lines indicate the $p_{0}$ values corresponding to local significances of $1 \sigma, 2 \sigma, 3 \sigma$ and $4 \sigma$.


Figure 16: The signal strength parameter $\mu=\sigma / \sigma_{S M}$ obtained from a fit to the data is presented (a) for the combined fit to the 2011 and 2012 data samples and (b) for the expected value of $\mu$ as a function of $m_{H}$ when a SM Higgs signal with $m_{H}=125 \mathrm{GeV}$ is injected.


Figure 17: Best fit values for $\mu$ and $m_{H}$, and likelihood ratio contours that, in the asymptotic limit, correspond to $68 \%$ and $95 \%$ level contours in the ( $\mu, m_{H}$ ) plane.

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## A Auxiliary material



Figure 18: Invariant mass of the four leptons, combining all final states, demonstrating the singleresonant peak $p p \rightarrow Z \rightarrow 4 \ell$. To improve the acceptance the following modifications were performed to the nominal analysis: the requirement on $m_{12}$ is relaxed to $30 \mathrm{GeV}<m_{12}<106 \mathrm{GeV}$, the requirement on $m_{34}$ is relaxed to $5 \mathrm{GeV}<m_{34}<115 \mathrm{GeV}$, and the $p_{\mathrm{T}}$ requirement on the softest muon was relaxed to $p_{\mathrm{T}}>4 \mathrm{GeV}$. For $4 \mu$ events, the requirement on the third muon is $p_{\mathrm{T}}>8 \mathrm{GeV}$. The data are shown for (a) $\sqrt{s}=8 \mathrm{TeV}$, (b) $\sqrt{s}=7 \mathrm{TeV}$ and (c) combined.


Figure 19: Ratio of the isolation and impact parameter efficiencies between data and simulation, estimated with the Tag \& Probe method, using (a) $Z \rightarrow \mu \mu$ and (b) $Z \rightarrow e e$ events.


Figure 20: Invariant mass distributions of the lepton pairs in the control sample defined by a $Z$ boson candidate and an additional same-flavour lepton pair, for the $\sqrt{s}=8 \mathrm{TeV}$ and $\sqrt{s}=7 \mathrm{TeV}$ datasets combined. The sample is divided according to the flavour of the additional lepton pair. In (a) the $m_{12}$ and in (c) the $m_{34}$ distributions are presented for $\ell \ell+\mu \mu$ events. In (b) the $m_{12}$ and in (d) the $m_{34}$ distributions are presented for $\ell \ell+e e$ events. The kinematic selection of the analysis is applied. Isolation and impact parameter significance requirements are applied to the first lepton pair only. The MC is normalized to the data driven background estimations.


Figure 21: The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates compared to the background expectation for the $80-250 \mathrm{GeV}$ mass range for the (a) $\sqrt{s}=8 \mathrm{TeV}$, (b) $\sqrt{s}=$ 7 TeV and (c) combined datasets. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown.


Figure 22: The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates for the combination of both analyses, compared to the background expectation. The $\sqrt{s}=8$ and $\sqrt{s}=7 \mathrm{TeV}$ datasets are shown separately in (a) and (b), respectively, and combined in (c). The combined result in the range $80-600 \mathrm{GeV}$ is also shown (d). Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown.


Figure 23: The distribution of the four-lepton invariant mass, $m_{4 \ell}$, for the selected candidates for the combination of both analyses for the various sub-channels, (a) $4 \mu$, (b) $2 \mu 2 e$, (c) $2 e 2 \mu$, (d) $4 e$, compared to the background expectation for the $80-250 \mathrm{GeV}$ mass range. Error bars represent $68.3 \%$ central confidence intervals. The signal expectation for several $m_{H}$ hypotheses is also shown.


Figure 24: Observed local $p_{0}$, the probability that the background fluctuates to the observed number of events or higher, for each analysis sub-channel, and for their combination. Dashed curves show the expected median local $p_{0}$ for the signal hypothesis when tested at $m_{H}$; (a) $2012(\sqrt{s}=8 \mathrm{TeV})$ data, (b) $2011(\sqrt{s}=7 \mathrm{TeV})$ data.


Figure 25: Observed local $p_{0}$, the probability that the background fluctuates to the observed number of events or higher, separating the two analyses with sub-leading muons ( $\ell \ell \mu \mu)$ from the two analyses with sub-leading electrons (८८ee); the black line shows the combined result. Dashed curves show the expected median local $p_{0}$ for the signal hypothesis when tested at $m_{H}$; (a) low mass region, (b) full mass range.


Figure 26: Observed local $p_{0}$, the probability that the background fluctuates to the observed number of events or higher, before and after the application of a $Z$ mass constraint. Dashed curves show the expected median local $p_{0}$ for the signal hypothesis when tested at $m_{H}$; (a) low mass region, (b) full mass range.


Figure 27: The observed local $p_{0}$, the probability that the background fluctuates to the observed number of events or higher, is shown as solid lines. The dashed curve shows the expected median local $p_{0}$ for the signal hypothesis when tested at $m_{H}$. (a) compares the local $p_{0}$ for the $\sqrt{s}=8 \mathrm{TeV}$ and the $\sqrt{s}=7 \mathrm{TeV}$ data samples; (b) shows the effect of allowing the irreducible background normalisation to float freely in the fit, for the $\sqrt{s}=8 \mathrm{TeV}$ data sample. The horizontal dashed lines indicate the $p_{0}$ values corresponding to local significances of $1 \sigma, 2 \sigma, 3 \sigma$ and $4 \sigma$.


Figure 28: Shape comparison of the $m_{4 \ell}$ distribution used for the $Z+j$ jets and $t \bar{t}$ contributions, in a control region where the sub-leading di-lepton fails either the isolation or the impact parameter significance requirements of the analysis, for both the $\sqrt{s}=7 \mathrm{TeV}$ and $\sqrt{s}=8 \mathrm{TeV}$ data samples.

## B Event Displays

## B. 1 EventNumber: 82614360 RunNumber: 203602



Figure 29: Event display of a $4 e$ candidate. EventNumber: 82614360 RunNumber: $203602 m_{4 \ell}=$ $124.6 \mathrm{GeV} . m_{12}=70.6 \mathrm{GeV}, m_{34}=44.7 \mathrm{GeV} . e_{1}: p_{\mathrm{T}}=24.9 \mathrm{GeV}, \eta=-0.33, \phi=1.98$. $e_{2}: p_{\mathrm{T}}=53.9 \mathrm{GeV}, \eta=-0.40, \phi=1.69 . e_{3}: p_{\mathrm{T}}=61.9 \mathrm{GeV}, \eta=-0.12, \phi=1.45 . e_{4}:$ $p_{\mathrm{T}}=17.8 \mathrm{GeV}, \eta=-0.51, \phi=2.84$.


Figure 30: Event display of a $4 e$ candidate. EventNumber: 82614360 RunNumber: $203602 m_{4 \ell}=$ $124.6 \mathrm{GeV} . m_{12}=70.6 \mathrm{GeV}, m_{34}=44.7 \mathrm{GeV} . e_{1}: p_{\mathrm{T}}=24.9 \mathrm{GeV}, \eta=-0.33, \phi=1.98$. $e_{2}: p_{\mathrm{T}}=53.9 \mathrm{GeV}, \eta=-0.40, \phi=1.69 . e_{3}: p_{\mathrm{T}}=61.9 \mathrm{GeV}, \eta=-0.12, \phi=1.45 . e_{4}:$ $p_{\mathrm{T}}=17.8 \mathrm{GeV}, \eta=-0.51, \phi=2.84$.

## B. 2 EventNumber: 82599793 RunNumber: 204769



Figure 31: Event display of a $4 \mu$ candidate. EventNumber: 82599793 RunNumber: $204769 m_{4 \ell}=$ $123.5 \mathrm{GeV} . m_{12}=84 \mathrm{GeV}, m_{34}=34.2 \mathrm{GeV} . \mu_{1}: p_{\mathrm{T}}=37.8 \mathrm{GeV}, \eta=0.61 \phi=1.46 . \mu_{2}$ : $p_{\mathrm{T}}=29.2 \mathrm{GeV}, \eta=-0.95, \phi=-2.47 . \mu_{3}: p_{\mathrm{T}}=10.3 \mathrm{GeV}, \eta=0.62 \phi=-1.41 . \mu_{4}: p_{\mathrm{T}}=$ $32.6 \mathrm{GeV} \eta=-0.16$, $\phi=2.85$.

## B. 3 EventNumber: 71402630 RunNumber: 204769



Figure 32: Event display of a $4 \mu$ candidate. EventNumber: 71902630 RunNumber: $204769 m_{4 \ell}=$ $125.1 \mathrm{GeV} . m_{12}=86.3 \mathrm{GeV}, m_{34}=31.6 \mathrm{GeV} . \mu_{1}: p_{\mathrm{T}}=36.1 \mathrm{GeV}, \eta=1.29, \phi=1.33$. $\mu_{2}: p_{\mathrm{T}}=47.5 \mathrm{GeV}, \eta=0.69, \phi=-1.65 . \mu_{3}: p_{\mathrm{T}}=26.4 \mathrm{GeV}, \eta=0.47, \phi=-2.51 . \mu_{4}:$ $p_{\mathrm{T}}=71.7 \mathrm{GeV}, \eta=1.85, \phi=1.65$.


Figure 33: Event display of a $4 \mu$ candidate. EventNumber: 71902630 RunNumber: $204769 m_{4 \ell}=$ $125.1 \mathrm{GeV} . m_{12}=86.3 \mathrm{GeV}, m_{34}=31.6 \mathrm{GeV} . \mu_{1}: p_{\mathrm{T}}=36.1 \mathrm{GeV}, \eta=1.29, \phi=1.33$. $\mu_{2}: p_{\mathrm{T}}=47.5 \mathrm{GeV}, \eta=0.69, \phi=-1.65 . \mu_{3}: p_{\mathrm{T}}=26.4 \mathrm{GeV}, \eta=0.47, \phi=-2.51 . \mu_{4}:$ $p_{\mathrm{T}}=71.7 \mathrm{GeV}, \eta=1.85, \phi=1.65$.

## B. 4 EventNumber: 12611816 RunNumber: 205113



Figure 34: Event display of a $2 e 2 \mu$ candidate. EventNumber: 12611816 RunNumber: $205113 m_{4 \ell}=$ $123.9 \mathrm{GeV} . m_{12}=87.9 \mathrm{GeV}, m_{34}=19.6 \mathrm{GeV} . e_{1}: p_{\mathrm{T}}=18.7 \mathrm{GeV}, \eta=-2.45, \phi=1.68 . e_{2}$ : $p_{\mathrm{T}}=75.96 \mathrm{GeV}, \eta=-1.16, \phi=-2.13 . \mu_{3}: p_{\mathrm{T}}=19.6 \mathrm{GeV}, \eta=-1.14, \phi=-0.87 . \mu_{4}:$ $p_{\mathrm{T}}=7.9 \mathrm{GeV}, \eta=-1.13, \phi=0.94$.

## ATLAS NOTE

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# Observation of an Excess of Events in the Search for the Standard Model Higgs boson with the ATLAS detector at the LHC 

The ATLAS Collaboration


#### Abstract

A preliminary combined search for the Standard Model Higgs boson with the ATLAS detector at the LHC is presented. The $p p$ collisions datasets used correspond to integrated luminosities of $4.6 \mathrm{fb}^{-1}$ to $4.9 \mathrm{fb}^{-1}$ at $\sqrt{s}=7 \mathrm{TeV}$ in 2011 and $5.8 \mathrm{fb}^{-1}$ to $5.9 \mathrm{fb}^{-1}$ at $\sqrt{s}=$ 8 TeV in 2012. Searches for $H \rightarrow \gamma \gamma, H \rightarrow Z Z^{(*)}, H \rightarrow W W^{(*)}, H \rightarrow b \bar{b}$, and $H \rightarrow \tau^{+} \tau^{-}$ have been performed on the 2011 data, while only the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$ searches are improved compared to previous analyses and use both the 2011 and 2012 data. The Standard Model Higgs boson is excluded at the $95 \%$ confidence level for masses in the range 110 GeV to 122.6 GeV and 129.7 GeV to 558 GeV . An excess of events is observed for a Higgs boson mass hypothesis near 126.5 GeV . The local significance of this excess is $5.0 \sigma$, where the expected significance in the presence of a Standard Model Higgs boson for that mass hypothesis is $4.6 \sigma$.


## 1 Introduction

Based on $p p$ collision data taken in 2011 at $\sqrt{s}=7 \mathrm{TeV}$, the ATLAS Collaboration reported an indication of an excess for Standard Model (SM) Higgs boson with a mass near $\sim 126.5 \mathrm{GeV}$ with a local significance of 2.9 standard deviations $(\sigma)[1]$. The global probability for the background to produce an excess at least as significant anywhere in the entire explored Higgs boson mass range of $110-600 \mathrm{GeV}$ was estimated to be $\sim 15 \%$. The mass ranges from 110.0 GeV to $117.5 \mathrm{GeV}, 118.5 \mathrm{GeV}$ to 122.5 GeV , and 129 GeV to 539 GeV were excluded at $95 \%$ confidence level (CL). The CMS collaboration performed a similar analysis of data collected in 2011, and found an excess corresponding to a local significance of $2.8 \sigma$ for $m_{H} \sim 125 \mathrm{GeV}$ [2]. The CDF and D 0 collaborations at the Tevatron have also reported an excess in the low mass region, in their combined searches for the SM Higgs boson in $p \bar{p}$ collisions [3]. The combined LEP limit [4] excludes a SM Higgs boson with a mass below 114.4 GeV at $95 \%$ CL.

These results have made the remaining mass region around 125 GeV the primary focus of the Higgs searches. This note describes the preliminary results from an improved analysis of the 2011 data and the additional 2012 data collected at $\sqrt{s}=8 \mathrm{TeV}$.

In the Standard Model [5-7], electroweak symmetry breaking is achieved via the Higgs mechanism, which results in a new particle referred to as the Higgs boson [8--13]. The Higgs boson mass, $m_{H}$, is a free parameter of the SM. However, for a given $m_{H}$ hypothesis, the production cross sections and branching ratios can be predicted. Searches for the Higgs boson in ATLAS are currently performed for twelve Higgs boson decay modes, taking into account subsequent decays of vector bosons and tau leptons. These channels are further subdivided according to lepton flavor, the presence of additional jet activity, kinematic regions, and other experimental factors in order to enhance the sensitivity. An overview of the channels is given in Table 1.

By July 2012, the LHC delivered to ATLAS $6.6 \mathrm{fb}^{-1}$ of $p p$ collisions at a center-of-mass energy of 8 TeV of which $6.2 \mathrm{fb}^{-1}$ were collected. In general, the increase in center-of-mass energy, with respect to the 7 TeV data taken in 2011, increases the signal production cross sections more than those of the backgrounds in all channels. The resulting increase in sensitivity of the analyses due to the increase in energy is equivalent to an increase in integrated luminosity of approximately 15-20\%. During 2012, the instantaneous luminosity reached record levels of approximately $7 \cdot 10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$, almost double the peak luminosity of 2011 with the same 50 ns bunch spacing. The increased luminosity thus came at the expense of an unprecedented number of $p p$ collisions per bunch crossing (pile-up), where the peak number of collisions corresponded to about 30 on average.

Due to the challenging running conditions of 2012, only the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$ channels, the two analyses most robust against pile-up, have been updated so far. The analysis of the 2011 data in these two channels has also been updated to benefit from improvements that have been made since the published result, which enhance the sensitivity to the SM Higgs boson. For $m_{H}=126.5 \mathrm{GeV}$ the expected significance in the presence of a SM from these two channels combined improves by $\sim 25 \%$ with respect to the results presented in Ref. [1]. All the other channels are unchanged with respect to Ref. [1].

## 2 Additions and Updates to 2011 Combination

## $2.1 H \rightarrow \gamma \gamma$

The $H \rightarrow \gamma \gamma$ search is carried out for $m_{H}$ hypotheses between 110 GeV and 150 GeV . The datasets used correspond to an integrated luminosity of $4.9 \mathrm{fb}^{-1}$ of $p p$ collisions collected at $\sqrt{s}=7 \mathrm{TeV}$ in 2011 and $5.9 \mathrm{fb}^{-1}$ of $p p$ collisions taken at $\sqrt{s}=8 \mathrm{TeV}$ in 2012 [14]. For this improved 2011 data analysis, the photon identification has been updated to use a neural network algorithm combining variables related

Table 1: Summary of the individual channels entering the combination. The transition points between separately optimized $m_{H}$ regions are indicated when applicable. The symbols $\otimes$ and $\oplus$ represent direct products or sums over sets of selection requirements.

| Higgs Decay | Subsequent Decay | Sub-Channels | $\begin{gathered} m_{H} \text { Range } \\ {[\mathrm{GeV}]} \end{gathered}$ | $\begin{aligned} & \int \mathrm{L} d t \\ & {\left[\mathrm{fb}^{-1}\right]} \end{aligned}$ | Ref. |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $2011 \sqrt{s}=7 \mathrm{TeV}$ |  |  |  |  |  |
| $H \rightarrow \gamma \gamma$ | - | 9 sub-channels $\left\{p_{\mathrm{T}_{t}} \otimes \eta_{\gamma} \otimes\right.$ conversion $\} \oplus\{2$-jets $\}$ | 110-150 | 4.8 | [14] |
| $H \rightarrow Z Z^{(*)}$ | $\ell \ell \ell^{\prime} \ell^{\prime}$ | $\{4 e, 2 e 2 \mu, 2 \mu 2 e, 4 \mu\}$ | 110-600 | 4.8 | [15] |
|  | $\ell \ell \nu \bar{v}$ | $\{e e, \mu \mu\} \otimes\{$ low, high pile-up $\}$ | 200-280-600 | 4.7 | 16 |
|  | $\ell \ell q \bar{q}$ | $\{b$-tagged, untagged $\}$ | 200-300-600 | 4.7 | 17 |
| $H \rightarrow W W^{(*)}$ | $\ell \nu \ell v$ | $\{e e, e \mu, \mu \mu\} \otimes\{0$-jets, 1-jet, 2-jets $\} \otimes$ low, high pile-up $\}$ | 110-200-300-600 | 4.7 | 18 |
|  | $\ell v q \bar{q}^{\prime}$ | $\{e, \mu\} \otimes\{0$-jets, 1-jet, 2-jets $\}$ | 300-600 | 4.7 | [19] |
| $H \rightarrow \tau^{+} \tau^{-}$ |  | $\{e \mu\} \otimes\{0$-jets $\} \oplus\{\ell \ell\} \otimes\{1$-jet, 2-jets, $V H\}$ | 110-150 | 4.7 | 20] |
|  | $\tau_{\text {lep }} \tau_{\text {had }}$ | $\begin{gathered} \{e, \mu\} \otimes\{0 \text {-jets }\} \otimes\left\{E_{\mathrm{T}}^{\text {miss }}<20 \mathrm{GeV}, E_{\mathrm{T}}^{\text {miss }} \geq 20 \mathrm{GeV}\right\} \\ \oplus\{e, \mu\} \otimes\{1 \text {-jet }\} \oplus\{\ell\} \otimes\{2 \text {-jets }\} \end{gathered}$ | 110-150 | 4.7 |  |
|  | $\tau_{\text {had }} \tau_{\text {had }}$ | \{1-jet $\}$ | 110-150 | 4.7 |  |
| $V H \rightarrow b \bar{b}$ | $Z \rightarrow \nu \bar{v}$ | $E_{\mathrm{T}}^{\text {miss }} \in\{120-160,160-200, \geq 200 \mathrm{GeV}\}$ | 110-130 | 4.6 | [21] |
|  | $W \rightarrow \ell v$ | $p_{\mathrm{T}}^{W} \in\{<50,50-100,100-200, \geq 200 \mathrm{GeV}\}$ | 110-130 | 4.7 |  |
|  | $Z \rightarrow \ell \ell$ | $p_{\mathrm{T}}^{\mathrm{Z}} \in\{<50,50-100,100-200, \geq 200 \mathrm{GeV}\}$ | 110-130 | 4.7 |  |
| $2012 \sqrt{s}=8 \mathrm{TeV}$ |  |  |  |  |  |
| $H \rightarrow \gamma \gamma$ | - | 9 sub-channels $\left\{p_{\mathrm{T}_{t}} \otimes \eta_{\gamma} \otimes\right.$ conversion $\} \oplus\{2$-jets $\}$ | 110-150 | 5.9 | [14 |
| $H \rightarrow Z Z^{(*)}$ | $\ell \ell \ell^{\prime} \ell^{\prime}$ | $\{4 e, 2 e 2 \mu, 2 \mu 2 e, 4 \mu\}$ | 110-600 | 5.8 | [15] |

to the shape of the shower in the electromagnetic calorimeter. For the 2012 data analysis, a cut-based identification algorithm is used. The analysis in this channel separates events into ten independent categories of varying sensitivity. Similarly to the analysis of Ref. [22], the categorization is based on the pseudorapidity of each photon, whether it was reconstructed as a converted or unconverted photon, and the momentum component of the diphoton system transverse to the diphoton thrust axis $\left(p_{\mathrm{T}_{t}}\right)$.

An additional two-jets category, specifically aimed at selecting events produced in the vector boson fusion (VBF) process, has been added to the analysis for both 2011 and 2012. In this category, events are required to have at least two hadronic jets with pseudorapidities $\left|\eta_{\text {jet }}\right|<4.5$ and transverse momenta in excess of 25 GeV . For the 2012 data sample, the minimum $p_{\mathrm{T}}^{\text {jet }}$ requirement is raised to 30 GeV for forward jets ( $2.5<\left|\eta_{\text {jet }}\right|<4.5$ ). The two jets are further required to have a large difference in pseudorapidity $\left(\left|\Delta \eta_{j j}\right|>2.8\right)$ and a large reconstructed invariant mass $\left(m_{j j}>400 \mathrm{GeV}\right)$. Jets in the acceptance of the inner tracking system are required to have more than $75 \%$ of their associated track momentum matched to the primary vertex. The azimuthal angle difference between the dijet and the diphoton systems is required to be larger than 2.6.

For all categories the diphoton invariant mass distribution is fitted to estimate the background and used as a discriminating variable to distinguish signal and background. The mass resolution is approximately 1.7 GeV for $m_{H} \sim 126.5 \mathrm{GeV}$, varying slightly by category. A detailed description of the $H \rightarrow \gamma \gamma$ analysis updates is reported in Ref. [14].

## 2.2 $H \rightarrow Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$

The $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$search is performed for $m_{H}$ hypotheses in the mass range between 110 GeV to 600 GeV . The datasets correspond to an integrated luminosities of $4.8 \mathrm{fb}^{-1}$ and $5.8 \mathrm{fb}^{-1}$ of $p p$ for 2011 and 2012, respectively [15]. The main irreducible $Z Z^{(*)}$ background is estimated using a Monte Carlo simulation. The reducible $Z+$ jets background, which has an impact mostly for low four-lepton invariant masses, is estimated from control regions in the data obtained by loosening the isolation and
impact parameter requirements placed on the sub-leading pair of leptons. The top-quark ( $t \bar{t}$ ) background normalization is simultaneously derived in this control region, and is validated in a separate top-enriched control region in which Z candidates are excluded. The events are categorized according to the lepton flavor combinations. The electron identification criteria have been reoptimized and the muon selection has been complemented with muons reconstructed exclusively in the muon system and muons reconstructed from tracks in the inner detector associated with energy deposits in the calorimeter compatible with minimum ionizing particles. The invariant mass of the lepton pair which is closest in mass to the Z-boson mass is required to be between $50 \mathrm{GeV}-106 \mathrm{GeV}$. The invariant mass of the other lepton pair is required to be smaller than 115 GeV and larger than a threshold ranging from 17.5 GeV to 50 GeV , depending on the reconstructed invariant four-leptons mass. A $J / \psi$ veto is applied on events with same flavor and opposite sign leptons with invariant mass smaller than 5 GeV . Several criteria have been reoptimized, including the transverse momentum of the three leading leptons, the impact parameter significance of all leptons, the calorimeter and track isolation, and the angular separation between the leptons. In addition, a kinematic fit, taking into account the natural width of the $Z$ boson and the energy and momentum resolution, improves the reconstructed Higgs boson mass resolution by $\sim 10 \%$. For $m_{4 l}<190 \mathrm{GeV}$, the $Z$ boson mass constraint is only used for the di-lepton pair with highest invariant mass, as one pair must originate from an off-shell $Z$ boson. Each of the four combinations of lepton flavor are treated as independent sub-channels. The mass resolutions are approximately $1.5 \%$ in the four-muon channel and $2 \%$ in the four-electron channel for $m_{H} \sim 120 \mathrm{GeV}$. The four-lepton invariant mass is used as a discriminating variable. A detailed description of the analysis updates in this channel is given in Ref. [15].

### 2.3 Systematic Uncertainties

Systematic uncertainties and the treatment of their correlations are unchanged with respect to Ref. [1] for all channels other than $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$. The systematic uncertainties in the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$channels have been estimated for both the 2011 and 2012 LHC running conditions. The treatment of systematic uncertainties associated with electron and photon energy scales has been updated to a more detailed model improving the treatment of correlations between electrons, converted photons, and unconverted photons.

Individual sources of systematic uncertainty affecting both 2011 and 2012 data are taken as fully correlated. The $\pm 3.9 \%$ uncertainty on the measurement of the integrated luminosity for 2011 data is considered uncorrelated with the $\pm 3.6 \%$ uncertainty on the measurement of the integrated luminosity in the 2012 data. Furthermore, the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$analyses now use an updated measurement of the integrated luminosity in 2011, which is $1.5 \%$ lower than the previous measurement with an improved uncertainty of $\pm 1.8 \%$ [?]. Since the leading uncertainties in the two estimates of the 2011 integrated luminosity arise from different sources the two estimates are treated as uncorrelated. A detailed review of all systematic uncertainties in the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$analyses is given in Refs. [14, 15].

## 3 Results

For each Higgs boson mass hypothesis the parameter of interest is the overall signal strength factor $\mu$, which acts as a scale factor to the total rate of signal events. This global factor is used for all pairings of production cross sections and branching ratios. The signal strength is defined such that $\mu=0$ corresponds to the background-only model and $\mu=1$ corresponds to the SM Higgs boson signal. The combination procedure used herein and described in Refs. [1, 23, 25] is based on the profile likelihood ratio test statistic $\lambda(\mu)$ [26]. The test statistic extracts the information on the signal strength from the full likelihood including all the parameters describing the systematic uncertainties and their correlations, and is designed
to be powerful in the presence of a SM Higgs. Exclusion limits are based on the $C L_{s}$ prescription [27]; a value of $\mu$ is regarded as excluded at the $95 \% \mathrm{CL}$ when $C L_{s}$ is less than $5 \%$. The statistical procedures are performed in a scan over the hypothesized value of the Higgs boson mass, and $m_{H}$ is held fixed in the likelihood function.

The combined $95 \%$ CL exclusion limits on $\mu$ are shown in Fig. 1 as a function of $m_{H}$. These results are based on the asymptotic approximation [26]. This procedure has been validated using ensemble tests and a Bayesian calculation of the exclusion limits with a uniform prior on the signal cross section. Typically, these two alternative approaches agree with the expected results from asymptotic approximations to within a few percent.

The expected $95 \%$ CL exclusion region covers the $m_{H}$ range from 110 GeV to 582 GeV . The observed $95 \%$ CL exclusion regions are from 110 GeV to 122.6 GeV and 129.7 GeV to 558 GeV . The addition of the $2012 H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$analyses as well as the improvements to the analysis of 2011 data in these two channels bring a significant gain in sensitivity in the low-mass region with respect to the previous combined search [1]. Figure 2] shows the $C L_{s}$ values for $\mu=1$, where it can be seen that the regions between 111.7 GeV to 121.8 GeV and 130.7 GeV to 523 GeV are excluded at the $99 \% \mathrm{CL}$. The observed exclusion covers a large part of the expected exclusion range ( 113.0 GeV to 522 GeV ), with the exception of the low mass region between 121.8 GeV and 130.7 GeV .

An excess of events is observed near $m_{H} \sim 126.5 \mathrm{GeV}$ in the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$ channels, both of which provide fully reconstructed candidates with high resolution in invariant mass. The significance of an excess is quantified by the probability $\left(p_{0}\right)$ that a background-only experiment is more signal-like than that observed. The local $p_{0}$ probability is assessed for a fixed $m_{H}$ hypothesis and the equivalent formulation in terms of number of standard deviations is referred to as the local significance. The probability for a background-only experiment to produce a local significance of this size or larger anywhere in a given mass region is referred to as the global $p_{0}$. The corresponding reduction in the significance is referred to as the "trials factor" or "look-elsewhere effect" and is estimated using the prescription described in Refs. [24,28].

The observed local $p_{0}$ values calculated using the asymptotic approximation as a function of $m_{H}$ are shown in Fig. 3. The expected $p_{0}$ corresponds to the median $p_{0}$ in the presence of a SM Higgs boson signal at that mass. The corresponding significances are shown in Fig. 4. In order to validate the asymptotic approximation for such extremely small $p$-values, an importance sampling algorithm has been used.

The largest local significance for the combined 2011+2012 analysis is found for a SM Higgs boson mass hypothesis of $m_{H}=126.5 \mathrm{GeV}$, where it reaches $5.1 \sigma$, with an expected value in the presence of a SM Higgs boson signal at that mass of $4.6 \sigma$. For the 2012 data alone, the maximum local significance for the $H \rightarrow \gamma \gamma$ and $H \rightarrow \mathrm{ZZ}^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$channels combined is $4.0 \sigma$, which occurs at $m_{H}=127.0 \mathrm{GeV}$ (3.4 $\sigma$ expected).

The significance of the excess is mildly sensitive to energy scale systematic (ESS) uncertainties and resolution for photons and electrons. The muon energy scale systematic uncertainties are smaller and therefore neglected. The presence of these uncertainties, which affect the shape and position of the signal distributions, lead to a small deviation in the distribution of the test statistic from a chi-square distribution. Previously, the observed $p_{0}$ including these effects was estimated using ensemble tests; however, the very small $p_{0}$ values makes this impractical computationally.

Here, a new approach to correcting for the leading departure from the asymptotic chi-square distribution is employed. The procedure is motivated by the observation that in the limit of very large energy scale uncertainties, an invariant mass peak could occur almost anywhere with $m_{H}$ fixed. This is essentially equivalent to the situation where $m_{H}$ is allowed to float freely in the fit, which gives rise to the look-elsewhere effect. The procedure outlined in Ref. [24, 28], which follows from theoretical work in

Ref. [29], corrects the minimum local $p$-value to the global $p$-value via

$$
\begin{equation*}
p_{0}^{\text {global }}=p_{0}^{\min \text { local }}+N e^{-\left(q_{0}\left(m_{H}\right)-u\right) / 2} \tag{1}
\end{equation*}
$$

where $N$ is the average number of times the test statistic $q_{0}\left(m_{H}\right)$ crosses some fixed value $u$ while scanning $m_{H}$ in the range considered. This corresponds to replacing the fixed threshold $u$ in the equation above with $u\left(m_{H}\right)$, a parabolic form related to the assumed Gaussian distribution of the energy scale uncertainty. A generalization of the fixed $u$ result [30] can be used to find the expected number of times the test statistic $q_{0}\left(m_{H}\right)$ is greater than $u\left(m_{H}\right)$. In essence, the correction to the local $p$-value due to energy scale systematics is similar to a look-elsewhere effect correction in a small search range. The effective size of the range, however, depends on the details of how several components to the energy scale uncertainty affect the ten different $H \rightarrow \gamma \gamma$ channels and four $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$channels. The effective $N$ can be estimated by fitting the sum of a chi-square and a falling exponential to the distribution of the test statistic created with a large number of pseudo-experiments. This hybrid ensemble-asymptotic approach was validated with much larger samples of pseudo-experiments generated for the previous combination [1] and shown to accurately reproduce the $p$-values. The result of this procedure for the full combined $2011+2012$ model results in a local significance including energy scale systematics of $5.0 \sigma$.

The global significance for local excesses depends on the range of $m_{H}$ and the channels considered. The global significance for the combined search to have a $5.0 \sigma$ excess anywhere in the mass range $110-$ 600 GeV is estimated to be approximately $4.1 \sigma$, increasing to $4.3 \sigma$ in the range $110-150 \mathrm{GeV}$ which is the range of the $H \rightarrow \gamma \gamma$ search and approximately the mass range not excluded at the $99 \%$ CL by the LHC combined SM Higgs boson search [31] and the LEP electroweak limits on a Standard Model Higgs boson [4]. The global significance for the $4.0 \sigma$ excess in the 2012 combined search to occur in the range $110-130.7 \mathrm{GeV}$, which is not excluded by the 2011 combination at $99 \%$ confidence level, is approximately $3.1 \sigma$.

The best-fit value of $\mu$, denoted $\hat{\mu}$, is displayed for the combination of all channels in Fig. 5 as a function of the $m_{H}$ hypothesis. The bands around $\hat{\mu}$ illustrate the $\mu$ interval corresponding to $-2 \ln \lambda(\mu)<$ 1 and represent an approximate $\pm 1 \sigma$ variation. While the estimator $\hat{\mu}$ is allowed to be negative in Fig. 5 in order to illustrate the presence and extent of downward fluctuations, the $\mu$ parameter is bounded to ensure non-negative values of the probability density functions in the individual channels. Hence, for negative $\hat{\mu}$ values close to the boundary, the $-2 \ln \lambda(\mu)<1$ region does not reflect a calibrated $68 \%$ confidence interval. It should be noted that $\hat{\mu}$ does not directly provide information on the relative strength of the production modes, nor does its maximum value give an estimate of the mass of a potential signal.

The best fit values of the signal strength parameter for each channel independently and for the combination are illustrated in Fig. 7 for $m_{H}=126.5 \mathrm{GeV}$. The observed excess corresponds to $\hat{\mu}$ of approximately $1.2 \pm 0.3$ for $m_{H}=126.5 \mathrm{GeV}$ with all 2011 and 2012 channels combined. This signal strength is consistent with the SM Higgs boson hypothesis $\mu=1$.

Neither the $m_{H}$ value that minimizes $p_{0}$ nor the one that maximizes $\hat{\mu}$ are unbiased estimates of the SM Higgs boson mass $m_{H}$ as they are computed using a fixed $m_{H}$ hypothesis. The maximum likelihood estimate of $m_{H}$ from the combined likelihood remains subject to further studies; however, likelihood contours of $\left(\mu, m_{H}\right)$ in the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$channels are presented in Appendix A. The probability for a single Higgs boson-like resonance to produce mass peaks separated by larger than the amount observed in these two channels, allowing the signal strengths to vary independently, is about $20 \%$.

## 4 Conclusion

Searches for the SM Higgs boson have been performed in the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$ channels with the ATLAS experiment at the LHC using 5.8-5.9 $\mathrm{fb}^{-1}$ of $p p$ collisions collected at a center-
of-mass energy of 8 TeV . These 2012 results are combined with the earlier 2011 results [1] based on an integrated luminosity of 4.7-4.9 $\mathrm{fb}^{-1}$, including improved $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$ analyses.

The observed SM Higgs boson exclusion ranges at the $95 \% \mathrm{CL}$ are 110 GeV to 122.6 GeV and 129.7 GeV to 558 GeV , while masses between 110 GeV to 582 GeV are expected to be excluded at the 95\% CL.

A significant $5 \sigma$ excess of events is observed in the search for the Standard Model Higgs boson, dominated by the two channels with the highest mass resolutions. This observation provides evidence for a new, narrow resonance at a mass near 126.5 GeV . Although the combined result including all search channels is consistent with the production and decay of a Standard Model Higgs boson, more data are needed to assess the nature of this excess.


Figure 1: The observed (full line) and expected (dashed line) $95 \%$ CL combined upper limits on the SM Higgs boson production cross section divided by the Standard Model expectation as a function of $m_{H}$ in the full mass range considered in this analysis (a) and in the low mass range (b). The dashed curves show the median expected limit in the absence of a signal and the green and yellow bands indicate the corresponding $68 \%$ and $95 \%$ intervals.


Figure 2: The value of the combined $C L_{s}$ for $\mu=1$ (testing the Standard Model Higgs boson hypothesis) as a function of $m_{H}$ in the full mass range of this analysis (a) and in the low mass range (b). The expected $C L_{s}$ is shown in the dashed curves. The regions with $C L_{s}<\alpha$ are excluded at least at ( $1-\alpha$ ) CL. The $95 \%$ and $99 \%$ CL values are indicated as dashed horizontal lines.


Figure 3: The local probability $p_{0}$ for a background-only experiment to be more signal-like than the observation in the full mass range of this analysis (a) and in the low mass range (b) as a function of $m_{H}$. The dashed curves show the median expected local $p_{0}$ under the hypothesis of a Standard Model Higgs boson production signal at that mass. The horizontal dashed lines indicate the $p$-values corresponding to significances of $1 \sigma$ to $6 \sigma$. Energy scale systematics are not included; taking them into account leads to a small negative correction $\sim 0.1 \sigma$ near $m_{H}=126 \mathrm{GeV}$.


Figure 4: The same as Fig. 3 shown in terms of local significance. An excess (deficit) of events corresponds to a positive (negative) local significance. This presentation makes clear the magnitude of a local deficit of events, where the logarithmic scale in Fig. 3 compresses large values of $p_{0}$. The dashed curves show the median expected local $p_{0}$ under the hypothesis of a Standard Model Higgs boson production signal at that mass. The horizontal dashed lines indicate significances ranging from $-2 \sigma$ to $5 \sigma$. Energy scale systematics are not included; taking them into account leads to a small correction $\sim 0.1 \sigma$ near $m_{H}=126 \mathrm{GeV}$.


Figure 5: The combined best-fit signal strength $\hat{\mu}$ as a function of the Higgs boson mass hypothesis (a) in the full mass range of this analysis and (b) in the low mass range. The interval around $\hat{\mu}$ corresponds to a variation of $-2 \ln \lambda(\mu)<1$.


Figure 6: The evolution of the local probability $p_{0}$ and the best-fit signal strength $\hat{\mu}$ from the 2011 data, the 2012 data, and their combination.


Figure 7: Summary of the individual and combined best-fit values of the strength parameter for a Higgs boson mass hypothesis of 126.5 GeV .


Figure 8: Summary of the individual and combined best-fit values of the strength parameter for three sample Higgs boson mass hypotheses of $119 \mathrm{GeV}, 126.5 \mathrm{GeV}$ and 130 GeV .


Figure 9: Likelihood contours in ( $\mu, m_{H}$ ) for the $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$and $H \rightarrow \gamma \gamma$ channels including energy scale systematics are shown in panel (a). The comparison of the contours with (thick lines) and without (thin lines in lighter colors) energy scale systematics is shown in panel (b).

## Appendix A: Contours in $\left(\mu, m_{H}\right)$ for $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$

The results presented so far do not give any information about the range of masses consistent with a potential signal, because the statistical procedure is performed in a scan over $m_{H}$ with $m_{H}$ fixed in the likelihood as if it were known a priori. These shortcomings are addressed by considering various contours of the likelihood function.

In order to address the values of the signal strength and mass of a potential signal that are simultaneously consistent with the data, the following profile likelihood ratio is used:

$$
\begin{equation*}
\lambda\left(\mu, m_{H}\right)=\frac{L\left(\mu, m_{H}, \hat{\boldsymbol{\theta}}\left(\mu, m_{H}\right)\right)}{L\left(\hat{\mu}, \hat{m}_{H}, \hat{\boldsymbol{\theta}}\right)} \tag{2}
\end{equation*}
$$

were $\hat{\boldsymbol{\theta}}\left(\mu, m_{H}\right)$ is the conditional maximum likelihood estimate with $\mu$ and $m_{H}$ fixed. In the presence of a strong signal, this test statistic will produce closed contours about the best fit point $\left(\hat{\mu}, \hat{m}_{h}\right)$; while in the absence of a signal the contours will be upper limits on $\mu$ for all values of $m_{H}$.

Asymptotically, the test statistic $-2 \ln \lambda\left(\mu, m_{H}\right)$ is distributed as a $\chi^{2}$ distribution with two degrees of freedom. In particular, the $100(1-\alpha) \%$ confidence level contours are defined by $-2 \ln \lambda\left(\mu, m_{H}\right)<k_{\alpha}$, where $k_{\alpha}$ satisfies $P\left(\chi_{2}^{2}>k_{\alpha}\right)=\alpha$.

The $68 \%$ and $95 \%$ CL contours for the $H \rightarrow \gamma \gamma$ channel are shown in Fig 9 , where the asymptotic approximations have been validated with ensembles of pseudo-experiments. Similar contours for the $H \rightarrow \mathrm{ZZ}^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$channel are shown in Fig 9 , where the distribution of $-2 \ln \lambda\left(\mu, m_{H}\right)$ is not expected to have converged to the asymptotic distribution. These preliminary contours in the ( $\mu, m_{H}$ ) plane take into account uncertainty in the energy scale and resolution. The impact of these uncertainties is illustrated in Fig. 9 (b).

The probability for a single Higgs boson-like resonance to produce mass peaks separated by larger than the amount observed in these two channels, allowing the signal strengths to vary independently, is about $20 \%$.

## Appendix B: Individual Channels and Combined Results

The individual channels observed and expected results in terms of CL limits, local probability $p_{0}$ and the corresponding significance are shown in Fig. 10, Fig. 11, and Fig. 12. The expected only results are shown in Fig. 13, Fig. 14, and Fig. 15 ,


Figure 10: The observed (solid) and expected (dashed) $95 \%$ CL cross section upper limits for the individual search channels and the combination, normalized to the SM Higgs boson production cross section, as a function of the Higgs boson mass hypothesis; (a) for the full Higgs boson mass hypotheses range and (b) in the low mass range. The expected limits are those for the background-only hypothesis i.e. in the absence of a Higgs boson signal.


Figure 11: The local probability $p_{0}$ for a background-only experiment to be more signal-like than the observation, for individual channels and the combination; (a) in the full mass range of $110-600 \mathrm{GeV}$ and (b) in the low mass range of $110-150 \mathrm{GeV}$. The full curves give the observed individual and combined $p_{0}$. The dashed curves show the median expected value under the hypothesis of a SM Higgs boson signal at that mass. The horizontal dashed lines indicate the $p_{0}$ corresponding to significances of $1 \sigma, 2 \sigma, 3 \sigma$, $4 \sigma$ and $5 \sigma$.


Figure 12: The local significance in terms of standard deviations for individual channels and the combination; (a) in the full mass range of $110-600 \mathrm{GeV}$ and (b) in the low mass range of $110-150 \mathrm{GeV}$. The full curves give the observed individual and combined local significances. The dashed curves show the median expected value under the hypothesis of a SM Higgs boson signal at that mass.


Figure 13: The expected $95 \%$ CL cross section upper limits for the individual search channels and the combination, normalized to the SM Higgs boson production cross section, as a function of the Higgs boson mass hypothesis; (a) for the full Higgs boson mass hypotheses range and (b) in the low mass range. The expected limits are those for the background-only hypothesis i.e. in the absence of a Higgs boson signal.


Figure 14: The expected local probability $p_{0}$ for a background-only experiment to be more signal-like than the observation, for individual channels and the combination; (a) in the full mass range of 110600 GeV and (b) in the low mass range of $110-150 \mathrm{GeV}$. The horizontal dashed lines indicate the $p_{0}$ corresponding to significances of $1 \sigma$ to $5 \sigma$.


Figure 15: The expected local significance in terms of standard deviations for individual channels and the combination. (a) In the full mass range of $110-600 \mathrm{GeV}$ and (b) in the low mass range of $110-150 \mathrm{GeV}$.

## Appendix C: Results from 2012

The primary results are shown here for the combination of the $2012 H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$ search channels alone.


Figure 16: The observed (full line) and expected (dashed line) 95\% CL combined upper limits on the SM Higgs boson production cross section divided by the Standard Model expectation as a function of $m_{H}$ for the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$analysis on 2012 data. The dashed curve shows the median expected limit in the absence of a signal and the green and yellow bands indicate the corresponding $68 \%$ and $95 \%$ intervals.


Figure 17: The value of the combined $C L_{s}$ for $\mu=1$ (testing the Standard Model Higgs boson hypothesis) as a function of $m_{H}$ for the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$analysis on 2012 data. The regions with $C L_{s}<\alpha$ are excluded at least at $(1-\alpha) \mathrm{CL}$. The $95 \%$ and $99 \% \mathrm{CL}$ values are indicated as dashed lines.


Figure 18: The local probability $p_{0}$ for a background-only experiment to be more signal-like than the observation as a function of $m_{H}$ for the $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$analysis on 2012 data. The dashed curves show the median expected local $p_{0}$ under the hypothesis of a Standard Model Higgs boson production signal at that mass. The horizontal dashed lines indicate the $p$-values corresponding to significances of $1 \sigma$ to $5 \sigma$.


Figure 19: The same as Fig. 18 shown in terms of local significance. An excess (deficit) of events corresponds to a positive (negative) local significance. This presentation makes clear the magnitude of a local deficit of events, where the logarithmic scale in Fig. 18 compresses large values of $p_{0}$. The dashed curves show the median expected local $p_{0}$ under the hypothesis of a Standard Model Higgs boson production signal at that mass. The horizontal dashed lines indicate significances ranging from $-2 \sigma$ to $5 \sigma$. Energy scale systematics are not included.


Figure 20: The combined best-fit signal strength $\hat{\mu}$ as a function of the Higgs boson mass hypothesis for the combination of the $2012 H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$analysis. The interval around $\hat{\mu}$ corresponds to a variation of $-2 \ln \lambda(\mu)<1$.

## Appendix D: Alternative Combinations

In order to compare the results obtained in the high mass resolution channels, $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow$ $\ell^{+} \ell^{-} \ell^{+} \ell^{-}$, with those of low mass resolution $H \rightarrow W W^{(*)} \rightarrow \ell^{+} v \ell^{-} \bar{v}, H \rightarrow \tau^{+} \tau^{-}$and $H \rightarrow b \bar{b}$, a separate combination of these channels is performed. The results are illustrated in Fig. 21.


Figure 21: (a) The local probability $p_{0}$ for a background-only experiment to be more signal-like than the observation and (b) the $95 \%$ CL upper limit on the Standard Model Higgs boson production cross section divided by the SM expectation as a function of $m_{H}$ is indicated by the solid curves for the combination of the high mass resolution $H \rightarrow \gamma \gamma$ and $H \rightarrow Z Z^{(*)} \rightarrow \ell^{+} \ell^{-} \ell^{+} \ell^{-}$channels (red), the low mass resolution channels $H \rightarrow W W^{(*)} \rightarrow \ell^{+} v \ell^{-} \bar{v}, H \rightarrow \tau^{+} \tau^{-}$and $H \rightarrow b \bar{b}$ channels (blue), and all channels (black). The dashed curves show (a) the median expected $p_{0}$ value under the hypothesis of a SM Higgs boson signal at that mass and (b) the median expected limit in the absence of a signal. The green and yellow bands indicate the corresponding $68 \%$ and $95 \%$ intervals for the full combination.

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## ATLAS NOTE

August 30, 2012


# Observation of an Excess of Events in the Search for the Standard Model Higgs Boson in the $\boldsymbol{H} \rightarrow \boldsymbol{W} \boldsymbol{W}^{(*)} \rightarrow \ell \nu \ell v$ Channel with the ATLAS <br> Detector 

The ATLAS Collaboration


#### Abstract

A Standard Model Higgs boson search in the $H \rightarrow W W^{(*)} \rightarrow e v \mu \nu$ decay mode has been performed using proton-proton collision data corresponding to an integrated luminosity of $5.8 \mathrm{fb}^{-1}$ at a centre-of-mass energy of 8 TeV collected during 2012 with the ATLAS detector at the Large Hadron Collider. The search focuses on the mass region around 125 GeV , not previously excluded, where an excess of events over the expected background is observed corresponding to a local $p_{0}$-value of $6 \times 10^{-4}$ or 3.2 standard deviations. In a combined analysis of the 2012 data with the $4.7 \mathrm{fb}^{-1}$ of data acquired at $\sqrt{s}=7 \mathrm{TeV}$ in 2011, the observed excess in the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channel corresponds to a minimum local $p_{0}$ of $3 \times 10^{-3}$ or 2.8 standard deviations.


This note has been modified from the original version dated 17 July to correct and improve the presentation. The results of the analysis are unchanged. The systematic uncertainties given in Table 4 were for the expected signal and backgrounds without upper and lower $m_{\mathrm{T}}$ thresholds, and have been changed to the uncertainties with the $m_{\mathrm{T}}$ thresholds applied. The systematic uncertainty on the muon fake factor was incorrectly stated as $60 \%$; it is $40 \%$ and has been corrected. The single top and $Z \rightarrow 4 \ell$ cross sections have been corrected in Table 1. The uncertainty on the normalisation factor for the top background in the $H+2$-jet analysis now includes the statistical uncertainty from the number of events in the control region. The best-fit $\mu$ value is quoted at $m_{H}=126 \mathrm{GeV}$, not 125 GeV , for consistency with the published results. Finally, there have been some small modifications to clarify the text.

## 1 Introduction

The Standard Model (SM) of particle physics [1-3] has been tested by many experiments over the last four decades and has been shown to successfully describe high energy phenomena. However, the mechanism that breaks electroweak symmetry in the SM still remains to be confirmed experimentally. This mechanism [4-6], which gives mass to all massive elementary particles, predicts the existence of a scalar particle, the Higgs boson. It is the only elementary particle in the SM that has not yet been observed and the search for the Higgs boson is a centrepiece of the LHC physics programme.

Indirect limits on the Higgs boson mass of $m_{H}<158 \mathrm{GeV}$ at $95 \%$ confidence level (CL) have been set using global fits to precision electroweak results [7]. Direct searches at LEP and the Tevatron have excluded at $95 \%$ CL a SM Higgs boson with a mass below 114.4 GeV [8] and in the regions $147 \mathrm{GeV}<m_{H}<180 \mathrm{GeV}$ and $100 \mathrm{GeV}<m_{H}<103 \mathrm{GeV}$ [9], respectively.

The results of searches in various channels using $\sqrt{s}=7 \mathrm{TeV}$ data corresponding to an integrated luminosity of approximately $5 \mathrm{fb}^{-1}$ have been reported recently by the ATLAS Collaboration, excluding the mass ranges $112.9 \mathrm{GeV}-115.5 \mathrm{GeV}, 131 \mathrm{GeV}-238 \mathrm{GeV}$, and $251 \mathrm{GeV}-466 \mathrm{GeV}$ [10]; and by the CMS Collaboration, excluding the mass range from 127 GeV to 600 GeV [11]. Due to the narrow region remaining in $m_{H}$ after the exclusions made from the 2011 data, the hypothesis of $m_{H}=125 \mathrm{GeV}$ is used to characterise the signal for many aspects of the search presented here.

The $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$ channel (with $\ell=e, \mu$ ) is particularly sensitive in the mass range $120<$ $m_{H}<200 \mathrm{GeV}$. This channel can play an important role in the determination of the coupling of the Higgs boson to $W$ bosons. The branching ratio to $W W$ falls off with decreasing $m_{H}$ below $m_{H}=2 m_{W}$ but is still just over $20 \%$ at $m_{H}=125 \mathrm{GeV}$ [12], and the dilepton final state allows the selection of events with a favourable signal-to-background ratio. The leading backgrounds are continuum $W W \rightarrow$ $\ell \nu \ell \nu$ production and $t \bar{t}$ events in which both $W$ bosons decay to $\ell \nu$. Additional sources of background include Drell-Yan ( $p p \rightarrow Z / \gamma^{*} \rightarrow \ell \ell$ ), $W+$ jets, single top, $W\left(Z / \gamma^{(*)}\right.$ ), and $Z Z$ events.

The previous $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell v$ search results reported by the ATLAS collaboration used the full 2011 dataset, corresponding to $4.7 \mathrm{fb}^{-1}$ of proton-proton $(p p)$ collisions at $\sqrt{s}=7 \mathrm{TeV}$, and excluded a SM Higgs boson in the mass range $133 \mathrm{GeV}<m_{H}<261 \mathrm{GeV}$ at $95 \%$ CL [13]. A similar search has been performed by the CMS Collaboration [14]. The analysis described here uses a dataset collected between the beginning of April to the middle of June 2012, which after requiring that all detector components are fully functional, corresponds to $5.8 \mathrm{fb}^{-1}$ of $p p$ collision data at a centre-of-mass of 8 TeV . The production cross section of a Higgs boson with $m_{H}=125 \mathrm{GeV}$ increases by about $30 \%$ with the increase of the centre-of-mass energy of the Large Hadron Collider from 7 TeV to 8 TeV . The analysis methodology reported in Ref. [13] is mostly unchanged, but some selection criteria have been modified to reduce background contributions while coping with the higher instantaneous luminosity of the LHC in 2012. In particular, the data are affected by the occurrence of multiple $p p$ collisions per bunch crossing, referred to as "pile-up". In the 2011 data the average number of interactions per bunch crossing was around 10. In 2012, the average has increased to around 20 . This results in significantly larger Drell-Yan background to the same-flavour final states, due to an increased rate of fake missing transverse energy. Since the $e \mu$ final state provides the large majority of the sensitivity of the search, only this final state has been used in the analysis reported here. Finally, more stringent isolation criteria are applied, to further reduce the $W+$ jets background.

Motivated by the 2011 combined Higgs searches [10], the analysis procedure was modified to blind the kinematic region where a signal might be expected. Events passing the kinematic selection designed to isolate a signal from a SM Higgs boson with a mass between 110 and 140 GeV were excluded during the development of the 2012 analysis. The signal region data were unblinded once the agreement between data and the background model in the control regions corresponding to the
dominant backgrounds was judged to be reasonable.
In the last part of this document, the results obtained at $\sqrt{s}=8 \mathrm{TeV}$ with $5.8 \mathrm{fb}^{-1}$ of data are combined with the published $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell v$ results from the 2011 dataset.

## 2 Data and simulated samples

The data used for this analysis were collected in 2012 using the ATLAS detector, a multi-purpose particle physics experiment with a forward-backward symmetric cylindrical geometry and near $4 \pi$ coverage in solid angle [15]. ATLAS consists of an inner tracking detector surrounded by a thin superconducting solenoid, electromagnetic and hadronic calorimeters, and an external muon spectrometer incorporating large superconducting air-core toroid magnets. The combination of these systems provides charged particle measurements together with efficient and precise lepton measurements over the pseudorapidity ${ }^{1}$ range $|\eta|<2.5$. Jets are reconstructed over the full coverage of the calorimeters, $|\eta|<4.9$; this calorimeter coverage also provides a measurement of the missing transverse momentum $E_{\mathrm{T}}^{\text {miss }}$.

The data used for this analysis were collected using inclusive single-muon and single-electron triggers. The two main triggers require the transverse momentum of the lepton with respect to the beam line, $p_{\mathrm{T}}$, to exceed 24 GeV and that the lepton be isolated: the scalar sum of the $p_{\mathrm{T}}$ of charged particles within $\Delta R=\sqrt{\Delta \phi^{2}+\Delta \eta^{2}}=0.2$ of the lepton direction is required to be less than 0.12 and 0.10 times the lepton $p_{\mathrm{T}}$ for the muon and electron, respectively. Because of the detector geometry, the acceptance of the muon trigger is limited to $|\eta|<2.4$. The trigger efficiencies are measured as a function of $p_{\mathrm{T}}, \eta$, and data-taking period using $Z$ events. The efficiencies are approximately $90 \%$ for electrons, and $90 \%$ ( $70 \%$ ) for muons in the endcap (barrel).

In this analysis, the signal contributions considered include the dominant gluon fusion production process ( $g g \rightarrow H$, denoted as $g g \mathrm{~F}$ ), the vector-boson fusion production process ( $q q^{\prime} \rightarrow q q^{\prime} H$, denoted as VBF) and the Higgs-strahlung process ( $q q^{\prime} \rightarrow W H, Z H$, denoted as $\left.W H / Z H\right)$. The $t \bar{t} H$ production mechanism is negligible due to its smaller cross section. For the decay of the Higgs boson, only the $H \rightarrow W W^{(*)} \rightarrow e \nu \mu \nu$ mode is considered, including the small contributions from leptonic $\tau$ decays. The branching fraction for this decay as a function of $m_{H}$ is calculated using the Prophecy 4 F [30,31] program, with HDECAY also used in calculating the total width [32].

The signal cross section is computed to next-to-next-to-leading order (NNLO) [33-38] in QCD for the ggF process using the MSTW2008 PDF set [39]. Next-to-leading order (NLO) electroweak (EW) corrections are also applied [40,41], as well as QCD soft-gluon resummations up to next-to-next-toleading $\log$ (NNLL) [42]. These calculations are detailed in Refs. [43,44], and assume factorisation between the QCD and EW corrections.

Approximate NNLO QCD corrections [45] and full NLO QCD and EW corrections [46-48] and are used to calculate the cross sections for VBF signal production. The cross sections of the associated $W H / Z H$ production processes are calculated up to NNLO QCD corrections [49, 50] and NLO EW corrections [51].

The Monte Carlo (MC) generators used to model signal and background processes are listed in Table 1. For most processes, separate programs are used to generate the hard scattering process and to model the parton showering, hadronisation, and the underlying event. PYTHIA [28] or PYTHIA8

[^70]Table 1: MC generators used to model the signal and background processes, and the corresponding cross sections at $\sqrt{s}=8 \mathrm{TeV}$ (given $m_{H}=125 \mathrm{GeV}$ in the case of the signal processes). The ggF Higgs boson $p_{\mathrm{T}}$ spectrum in POWHEG [12] is tuned to agree with the prediction from HqT [16]. Finite heavy quark mass effects in the gluon-gluon production are also included [17]. The relevant single-top production channels ( $s$-channel and $W t$ ) are included. The number quoted for the inclusive $Z / \gamma^{*}$ process (also referred to in the text as the Drell-Yan process) is for generated dilepton invariant masses greater than 10 GeV . Kinematic criteria are also applied in the generation of $W(\rightarrow \ell v) \gamma$ events (the photon must have $p_{\mathrm{T}}>8 \mathrm{GeV}$ and be separated from the charged lepton by $\left.\Delta R=\sqrt{\left(\Delta \eta^{2}\right)+\left(\Delta \phi^{2}\right)}>0.25\right)$ and $W(\rightarrow \ell v) \gamma^{*}\left(\rightarrow \ell^{\prime} \ell^{\prime}\right)$ events (at least two leptons have $p_{T}$ larger than 5 GeV and $|\eta|<3$ for the $e e$ and $\mu \mu$ case, and $|\eta|<5$ for the $\tau \tau$ case). The $Z^{(*)} Z^{(*)} \rightarrow 4 \ell$ samples are generated with an invariant mass cut of $m_{\ell \ell}>4 \mathrm{GeV}$. For the $W Z^{(*)}$ and $W \gamma^{*}$ processes, MADGRAPH includes the interference between the $Z^{(*)}$ and the $\gamma^{*}$, and the boundary between the samples is at $m_{\ell \ell}=7 \mathrm{GeV}$. For the $W \gamma^{*}$ a lower invariant mass cut of $m_{\ell \ell}>2 m_{e}$ is applied. Leptonic decays of $W / Z$ bosons are always assumed, and the quoted cross sections include the branching ratios and are summed over lepton flavours. The exception is top quark production; for which inclusive cross sections are quoted.

| Process | Generator | $m_{H}(\mathrm{GeV})$ | $\sigma \cdot \mathrm{Br}(\mathrm{pb})$ |
| :--- | :--- | ---: | ---: |
| ggF | POWHEG [18]+PYTHIA8 [19] | 125 | 0.441 |
| VBF | POWHEG [20]+PYTHIA8 | 125 | $35 \cdot 10^{-3}$ |
| $W H / Z H$ | PYTHIA8 | 125 | $25 \cdot 10^{-3}$ |
| $q \bar{q} / g \rightarrow W W$ | MC@NLO [21]+HERWIG [22] | 5.68 |  |
| $g g \rightarrow W W$ | GG2WW [23]+HERWIG | 0.16 |  |
| $t \bar{t}$ | MC@NLO+HERWIG | 238 |  |
| $t W / t b$ | MC@NLO+HERWIG | 28 |  |
| $t q b$ | AcerMC [24]+PYTHIA | 88 |  |
| inclusive $W$ | ALPGEN [25]+HERWIG | $37 \cdot 10^{3}$ |  |
| inclusive $Z / \gamma^{*}$ | ALPGEN+HERWIG | $16 \cdot 10^{3}$ |  |
| $Z^{(*)} Z^{(*)} \rightarrow 4 l$ | POWHEG+PYTHIA8 | 0.73 |  |
| $W Z^{(*)}$ | MADGRAPH [26,27]+PYTHIA [28] | 1.54 |  |
| $W \gamma^{*}$ | MADGRAPH [29]+PYTHIA | 9.26 |  |
| $W \gamma$ | ALPGEN+HERWIG | 369 |  |

[19] are used for these latter three steps for the signal and some of the background processes. When HERWIG [22] is used for the hadronisation and parton showering the underlying event is modelled using JIMMY [52]. The MLM matching scheme [53] is used for the description of the $W+$ jets, $Z / \gamma^{*}+$ jets and $W \gamma$ processes. The cross sections for the $W \gamma$ and $W \gamma^{*} / W Z^{(*)}$ processes are normalised to the MCFM [54] NLO predictions. These normalisation factors (K-factors) are calculated to be 1.15 for $W \gamma, 1.3$ for $W \gamma^{*}\left(m_{\ell \ell}<7 \mathrm{GeV}\right)$ and 1.51 for $W Z^{(*)}\left(m_{\ell \ell}>7 \mathrm{GeV}\right)$.

The CT10 parton distribution function (PDF) set [55] is used for the POWHEG and MC@NLO samples, and CTEQ6L1 [56] is used for the ALPGEN, MadGraph, and PYTHIA8 samples. Acceptances and efficiencies are obtained from a full simulation [57] of the ATLAS detector using GEANT4 [58]. The simulation incorporates a model of the pile-up conditions in the 2012 data, including both the effects of multiple $p p$ collisions in the same bunch crossing ("in-time" pile-up) and in nearby bunch crossings ("out-of-time" pile-up).

## 3 Event selection

Events are required to have a primary vertex consistent with the beam spot position, with at least three associated tracks with $p_{\mathrm{T}}>400 \mathrm{MeV}$. Data quality criteria are applied to events in order to suppress non-collision backgrounds such as cosmic-ray muons, beam-related backgrounds, or noise in the calorimeters.
$H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell v$ candidates (with $\ell=e, \mu$ ) are pre-selected by requiring exactly two oppositely charged leptons of different flavours, with $p_{\mathrm{T}}$ thresholds of 25 GeV and 15 GeV for the leading and sub-leading lepton, respectively. Events are classified into two exclusive lepton channels depending on the flavour of the leading lepton: in the following, $e \mu(\mu e)$ will refer to events with a leading electron (muon). The dilepton invariant mass is required to be greater than 10 GeV . For muons, the range $|\eta|<2.5$ is used; for electrons, the range $|\eta|<2.47$ is used, with the region $1.37<|\eta|<1.52$, corresponding to the boundary between barrel and end-cap calorimeters, excluded.

Electron candidates are selected by applying a set of tight identification criteria using a combination of tracking and calorimetric information. The fine lateral and longitudinal segmentation of the calorimeter and transition radiation capability of the ATLAS detector have allowed the previous levels of electron performance [59] to be retained in the increased pile-up environment of the 2012 data taking. Muon candidates are identified by matching tracks reconstructed in the inner detector and in the muon spectrometer [60]. Requirements on the number of hits in all three components of the inner detector (pixels, SCT, and TRT) provide background rejection, particularly against pion/kaon decays-in-flight.

At least one of the selected leptons is required to match a triggering object. Leptons from heavyflavour decays and jets satisfying the lepton identification criteria are suppressed by requiring the leptons to be isolated: the scalar sum of the $p_{T}$ of charged particles and of the calorimeter energy deposits within $\Delta R=\sqrt{\Delta \phi^{2}+\Delta \eta^{2}}=0.3$ of the lepton direction (excluding the lepton itself) are each required to be less than $0.12-0.20$ times the lepton $p_{\mathrm{T}}$. The exact value differs between the trackand calorimeter-based criteria, between electrons and muons, and depend on the lepton $p_{\mathrm{T}}$.

Drell-Yan and QCD multijet events are suppressed by requiring large $E_{\mathrm{T}}^{\mathrm{miss}}$ [61]. The $E_{\mathrm{T}}^{\mathrm{miss}}$ is the magnitude of $\mathbf{E}_{\mathrm{T}}^{\mathrm{miss}}$, the opposite of the vector sum of the transverse momenta of the reconstructed objects, including muons, electrons, photons, jets, and clusters of calorimeter cells not associated with these objects. The quantity $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ used in this analysis is defined as: $E_{\mathrm{T}, \mathrm{rel}}^{\mathrm{miss}}=E_{\mathrm{T}}^{\mathrm{miss}} \sin \Delta \phi_{\mathrm{min}}$, with $\Delta \phi_{\min } \equiv \min \left(\Delta \phi, \frac{\pi}{2}\right)$. Here, $\Delta \phi$ is the minimum azimuthal angle between $\mathbf{E}_{\mathrm{T}}^{\text {miss }}$ and the leading lepton, the sub-leading lepton or any jet with $p_{\mathrm{T}}>25 \mathrm{GeV}$.

Compared to $E_{\mathrm{T}}^{\mathrm{miss}}$, the use of $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ increases the rejection of events with significant mismeasurement of a jet or a lepton, since in such events the direction in $\phi$ of the $\mathbf{E}_{\mathrm{T}}^{\mathrm{miss}}$ is correlated with the direction of the mismeasured object. Figure 1 shows the distribution of $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ in dilepton events passing all of the selection above, up to but not including the $E_{\mathrm{T} \text {,rel }}^{\mathrm{miss}}$ threshold. The threshold applied in this analysis is 25 GeV . Any multijet background present at this stage is included in the $W+$ jets background estimate. After the lepton isolation and $E_{\mathrm{T}, \text { rel }}^{\mathrm{miss}}$ requirements, the multijet background is negligible and the Drell-Yan background is much reduced. The Drell-Yan contribution becomes negligible after the topological selections, described later in this section, are applied.

Figure 1 shows the multiplicity distribution of jets reconstructed using the anti- $k_{t}$ algorithm [62], with distance parameter $R=0.4$, for all events satisfying the pre-selection criteria described above including the $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ requirement. Only jets with $p_{\mathrm{T}}>25 \mathrm{GeV}$ and $|\eta|<4.5$ are considered. The jet $p_{\mathrm{T}}$ threshold is increased to 30 GeV in the forward region $2.5<|\eta|<4.5$ to reduce the contribution from jets produced by pile-up. In order to reject jets that are produced in the central part of the detector by


Figure 1: $E_{\mathrm{T}, \text { rel }}^{\mathrm{miss}}(\mathrm{left})$ and multiplicity of jets (right) for events satisfying the pre-selection criteria described in the text. (No $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ requirement is applied in the $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ distribution.) The jet selection applied is $p_{T}^{j e t}>25 \mathrm{GeV}$ for $\left|\eta^{j e t}\right|<2.5$ and $p_{T}^{j e t}>30 \mathrm{GeV}$ for $2.5<\left|\eta^{j e t}\right|<4.5$. The lepton channels are combined. The hashed area indicates the total uncertainty on the background prediction. The $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The expected signal for a SM Higgs boson with $m_{H}=125 \mathrm{GeV}$ is superimposed.
pile-up interactions, a selection criterion is applied to each jet with $|\eta|<2.5$ on a quantity called the jet vertex fraction (JVF). The JVF is defined, using the charged tracks associated with a given jet, to be the $p_{\mathrm{T}}$ sum of the tracks originating from the primary vertex divided by the $p_{\mathrm{T}}$ sum of all of the tracks. Jets are required to have JVF $>0.5$. This selection was found to be robust against pile-up, based on studies of the dependence of the jet multiplicity on the number of reconstructed vertices in the $2012 Z+$ jet data. Figure 2 shows the ratio of $Z \rightarrow \mu \mu+1$-jet events to all $Z \rightarrow \mu \mu$ events as a function of the number of reconstructed primary vertices. The events are selected by applying the pre-selection criteria (excluding the $E_{\mathrm{T} \text {,rel }}^{\mathrm{miss}}$ requirement) with two muons and an additional requirement on the invariant mass ( $\left|m_{\mu \mu}-m_{Z}\right|<15 \mathrm{GeV}$ ) in order to select $Z$ events. No dependence is seen with the jet selection described above.

The background rate and composition depend significantly on the jet multiplicity, as does the signal topology. Without accompanying jets, the signal originates almost entirely from the ggF process and the background is dominated by $W W$ and Drell-Yan events. In contrast, when produced in association with two or more jets, the signal contains a much larger contribution from the VBF process and the background is dominated by $t \bar{t}$ production. To maximise the sensitivity, further selection criteria that depend on the jet multiplicity are applied to the pre-selected sample. The data are subdivided into $H+0$-jet, $H+1$-jet and $H+2$-jet channels according to the jet counting defined above (with the $H+2$-jet channel also including higher jet multiplicities at this stage). The different requirements for these channels are described in more detail below.

Due to spin correlations in the $W W^{(*)}$ system arising from the spin-0 nature of the SM Higgs boson and the V-A structure of the $W$ boson decay, the charged leptons tend to emerge from the interaction point in the same direction. This kinematic feature is exploited for all jet multiplicities by requiring that the azimuthal angular difference between the leptons, $\Delta \phi_{\ell \ell}$, be less than 1.8 radians, and that the dilepton invariant mass, $m_{\ell \ell}$, be less than 50 GeV for the $H+0$-jet and $H+1$-jet channels. For the $H+2$-jet channel, the $m_{\ell \ell}$ upper bound is increased to 80 GeV . The $m_{\ell \ell}$ distribution is somewhat harder


Figure 2: Ratio of $Z \rightarrow \mu \mu+1$-jet events to all $Z \rightarrow \mu \mu$ candidates as a function of the number of reconstructed primary vertices in the event. The selected events must pass the pre-selection criteria, excluding the $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ requirement, with the additional selection of $\left|m_{\mu \mu}-m_{Z}\right|<15 \mathrm{GeV}$. Only statistical uncertainties are included.
for the $H+2$-jet topology since the Higgs boson is more strongly boosted, reducing the alignment of the $W \mathrm{~s}$ and decorrelating the lepton directions.

In the $H+0$-jet channel, the magnitude $p_{\mathrm{T}}^{\ell \ell}$ of the transverse momentum of the dilepton system, $\mathbf{p}_{\mathrm{T}}^{\ell \ell}=\mathbf{p}_{\mathrm{T}}^{\ell 1}+\mathbf{p}_{\mathrm{T}}^{\ell 2}$, is required to be greater than 30 GeV . This improves the rejection of the Drell-Yan background.

In the $H+1$-jet channel, backgrounds from top quark decays are suppressed by rejecting events containing a jet identified as being consistent with originating from the decay of a $b$ or $c$ quark $(b-$ tagged jet), using a $b$-tagging algorithm based on a neural network that exploits the topology of weak decays of $b$ - and $c$-hadrons [63]. The algorithm is tuned to achieve an $85 \% b$-jet identification efficiency in $t \bar{t}$ events while yielding a light-jet tagging rate of approximately $11 \%$ [64]. The total transverse momentum, $p_{\mathrm{T}}^{\text {tot }}$, defined as the magnitude of the vector $\operatorname{sum} \mathbf{p}_{\mathrm{T}}^{\text {tot }}=\mathbf{p}_{\mathrm{T}}^{\ell 1}+\mathbf{p}_{\mathrm{T}}^{\ell 2}+\mathbf{p}_{\mathrm{T}}^{\mathrm{j}}+\mathbf{E}_{\mathrm{T}}^{\text {miss }}$, is required to be smaller than 30 GeV to suppress top background events that have additional jets with $p_{\mathrm{T}}$ below threshold. The $\tau \tau$ invariant mass, $m_{\tau \tau}$, is computed under the assumption that the reconstructed leptons are $\tau$ lepton decay products, that the neutrinos produced in the $\tau$ decays are collinear with the leptons [65], and that they are the only source of $E_{\mathrm{T}}^{\text {miss }}$. Events with $\left|m_{\tau \tau}-m_{Z}\right|<25 \mathrm{GeV}$ are rejected if the energy fractions carried by the putative visible decay products are positive (the collinear approximation does not always yield physical solutions).

The $H+2$-jet selection follows the $H+1$-jet selection described above (with the $p_{\mathrm{T}}^{\text {tot }}$ definition modified to include all selected jets). In addition, several additional jet-related criteria are applied to the two highest- $p_{\mathrm{T}}$ jets in the event, referred to as the "tag" jets. The tag jets must be separated in rapidity by a distance $\left|\Delta y_{\mathrm{jj}}\right|$ of at least 3.8. Events with an additional jet with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in between the tag jets $\left(y_{j 1}<y<y_{j 2}\right)$ are vetoed. Finally, the invariant mass of the two tag jets, $m_{\mathrm{jj}}$, must be at least 500 GeV .

A transverse mass variable, $m_{\mathrm{T}}$ [66], is used in this analysis to test for the presence of a signal for all jet multiplicities. This variable is defined as:

$$
m_{\mathrm{T}}=\sqrt{\left(E_{\mathrm{T}}^{\ell \ell}+E_{\mathrm{T}}^{\mathrm{miss}}\right)^{2}-\left|\mathbf{p}_{\mathrm{T}}^{\ell \ell}+\mathbf{E}_{\mathrm{T}}^{\mathrm{miss}}\right|^{2}}
$$

where $E_{\mathrm{T}}^{\ell \ell}=\sqrt{\left|\mathbf{p}_{\mathrm{T}}^{\ell \ell}\right|^{2}+m_{\ell \ell}^{2}}$. The statistical analysis of the candidate data uses a fit to the $m_{T}$ shape in the signal region data after the $\Delta \phi_{\ell \ell}$ requirement (see Section 6). The signal sensitivity for a SM Higgs
mass hypothesis $m_{H}$ can also be enhanced by selecting events with $m_{T}$ in the range $0.75 m_{H}<m_{T}<$ $m_{H}$, and this additional selection is used later in this document to illustrate the background model and the observed excess. The signal-to-background ratios after this selection for a SM Higgs boson with $m_{H}=125 \mathrm{GeV}$, with the added $m_{T}$ requirement, are about $0.14,0.19$, and 1.0 for the $H+0$-jet, $H+1$-jet, and $H+2$-jet selections, respectively.

## 4 Background normalisation and control samples

For the $H+0$-jet and $H+1$-jet analyses, the leading backgrounds from SM processes producing two isolated high- $p_{\mathrm{T}}$ leptons are $W W$ and top (in this note, "top" background always includes both $t \bar{t}$ and single top ( $t W, t b$, and $t q b$ ) unless explicitly stated otherwise). These are estimated using partially data-driven techniques based on normalising the MC predictions to the data in control regions dominated by the relevant background source. The $W+$ jets background is fully estimated from data for all jet multiplicities. Only the backgrounds from Drell-Yan, diboson processes other than $W W$, and the $W W$ background for the $H+2$-jet analysis are estimated using simulation.

The control and validation regions are defined by selections similar to those used in the signal region but with some criteria reversed or modified to obtain signal-depleted samples enriched in a particular background. The control regions for $W W$ and top are used to normalise the corresponding backgrounds in the fit, which helps reduce the sensitivity of the background predictions to the systematic uncertainties detailed in Section 5. The normalisation and $m_{T}$ shape of the $W+$ jets background are also derived from a control region and extrapolated into the signal region using a "fake factor" defined below. Same-sign dilepton events are produced primarily by the $W+j$ jets, $W \gamma^{(*)} / W Z^{(*)}$ and $Z^{(*)} Z^{(*)}$ processes. These events are thus used as a validation region to check those background predictions. The term "validation region" distinguishes these regions from the control regions, which are used to directly normalise the corresponding backgrounds.

Some control regions have significant contributions from backgrounds other than the targeted one, which introduces dependencies among the background estimates. These correlations are fully incorporated in the profile likelihood used to test the background-only hypothesis (see Section 6). In the following subsections, each background estimate is described after any others on which it depends. Because of this, the largest background ( $W W$ ) is described last.

## 4.1 $W+$ jets estimation and the same-sign validation sample

The $W+$ jets background contribution is estimated using a control sample of events in which one of the two leptons satisfies the identification and isolation criteria described in Section 3, and the other lepton (denoted "anti-identified") fails these criteria but satisfies a loosened selection. Anti-identified electrons satisfy loosened isolation requirements and must fail at least one electron identification requirement, which may be on the shower shape or track quality. For anti-identified muons, the calorimeter isolation requirement is loosened and the track isolation and transverse impact parameter requirements are removed. Further, the muon must not pass all of the muon identification criteria. Otherwise, events in this sample are required to pass all of the signal selection requirements. The dominant contribution to this background comes from $W+$ jets events in which a jet produces an object which is reconstructed as a lepton. This object may be either a true electron or muon from the decay of a heavy quark, or else, in the case of electrons, a product of the fragmentation incorrectly reconstructed as an isolated electron candidate. The purity of $W+$ jets events in the control region is about $90 \%$ in the electron channel and $70 \%$ in the muon channel.


Figure 3: Distribution of $m_{T}$ (left) and $\Delta \phi_{\ell \ell}$ (right) in the same-sign validation region after the $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ and zero jet requirements. The lepton flavours are combined. The signal shown is for $m_{H}=125 \mathrm{GeV}$. The hashed area indicates the total uncertainty on the background prediction.

The $W+$ jets background in the signal region is obtained by scaling the number of events in the data control sample by a "fake factor". The fake factor is defined as the ratio of the number of fully identified lepton candidates passing all selections to the number which are anti-identified. It is estimated as a function of the anti-identified lepton $p_{\text {T }}$ using an inclusive dijet data sample, after subtracting the residual contributions from leptons produced by leptonic $W$ and $Z$ decays. For this subtraction, the $W$ candidates are identified by requiring the transverse mass $m_{\mathrm{T}}^{W}=\sqrt{2 p_{\mathrm{T}}^{\ell} E_{\mathrm{T}}^{\mathrm{miss}} \cdot(1-\cos \Delta \phi)}$ to satisfy $m_{\mathrm{T}}^{W}>30 \mathrm{GeV}$. In this expression, $p_{\mathrm{T}}^{\ell}$ is the lepton transverse momentum and $\Delta \phi$ is the difference in azimuth between the lepton and $\mathbf{E}_{\mathrm{T}}^{\text {miss }}$ directions. The $Z$ candidates are identified as two opposite-sign leptons of the same flavour with $\left|m_{\ell \ell}-m_{Z}\right|<15 \mathrm{GeV}$, and need to be subtracted as part of the fake factor calculation even though only $e \mu$ candidates are selected in the signal region. The remaining lepton contamination, which includes $W \gamma$ and $W \gamma^{*} / W Z^{(*)}$ events, is subtracted using MC simulation.

The fake factor uncertainty is the main uncertainty on the $W+$ jets background contribution. It is dominated by differences in jet composition between dijet and $W+$ jets samples as observed in MC simulation, accounting also for differences between the heavy-flavour ( $b$ and $c$ quark) content of the simulated $W+$ jets events and what has been measured in data. The total systematic uncertainty on the fake factor also includes smaller contributions originating from trigger effects and the subtraction of the contamination from leptonic $W$ and $Z$ decays. The total relative uncertainty on this background is approximately $40 \%$ for the electron fakes and $40 \%$ for the muon fakes.

The processes producing the majority of same-sign dilepton events, $W+$ jets, $W \gamma^{(*)}, W Z^{(*)}$, and $Z^{(*)} Z^{(*)}$ are all backgrounds to $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu . W+\mathrm{jets}$ and $W \gamma^{(*)}$ are particularly important for the analysis optimised for a low Higgs boson mass hypothesis. Therefore the normalisation and kinematic features of same-sign dilepton events are used to validate these background predictions. Satisfactory agreement is observed overall, and example distributions, the $m_{\mathrm{T}}$ and $\Delta \phi_{\ell \ell}$ distributions of same-sign zero-jet events passing the preselection requirements, are shown in Fig. 3. The observed number of events is somewhat smaller than the estimated background, although the differences seen are well within the statistical and systematic uncertainties.

The $W \gamma$ background arises from the photon converting into a electron-positron pair, while the $W$ decay provides the muon and the $E_{\mathrm{T}}^{\mathrm{miss}}$ signatures. The simulation of the $W \gamma$ background is tested in a modified same-sign validation region in which the electron criteria that remove photon conversions are reversed. In this region, a high $W \gamma$ purity is obtained (approximately $80 \%$ ). The final estimate is
taken from MC simulation since there are insufficient data in the $W \gamma$ validation region to derive an accurate normalisation, but the agreement between data and MC is good within the large statistical uncertainty.

### 4.2 Top-quark control sample

The number of background events from top quark production in the $H+0$-jet signal region is normalised to the number of events satisfying the pre-selection criteria described in Section 3, namely, the selection up to but not including the jet multiplicity requirements. This sample is dominated by top quark events, as shown in Fig. 1. The small contribution of non-top backgrounds to this sample is estimated from simulation, except for the $W+$ jets contribution, which is estimated from data. The fraction $f_{0-\text { jet }}^{\mathrm{MC}}$ of top events in the preselected sample which pass the jet veto is initially estimated in simulation and then corrected using kinematic information from a second, $b$-tagged, control sample. Specifically, the correction uses the probability $P_{1}^{\mathrm{b}-\mathrm{tag}}$ for an event in the control sample to have no jets reconstructed in addition to the one that is tagged. Because $b$-tagging selects a nearly pure sample of top events, $P_{1}^{\mathrm{b}-\mathrm{tag}}$ can be calculated in both data and simulation. Then $f_{0-\mathrm{jet}}^{\mathrm{data}}$ is estimated by multiplying $f_{0-\text { jet }}^{\mathrm{MC}}$ by the ratio $\left(P_{1}^{\mathrm{b}-\mathrm{tag}, \mathrm{data}}\right)^{2} /\left(P_{1}^{\mathrm{b}-\mathrm{tag}, \mathrm{MC}}\right)^{2}$, exploiting the stability of the ratio $f_{0-\text { jet }} /\left(P_{1}^{\mathrm{b}-\mathrm{tag}}\right)^{2}$ with respect to experimental uncertainties and, to a lesser extent, assumptions about top event kinematics [67]. The efficiency for the remaining requirements on $p_{\mathrm{T}}^{\ell \ell}, m_{\ell \ell}$, and $\Delta \phi_{\ell \ell}$ is taken from simulation. The ratio of the resulting prediction to the one from simulation alone is $1.11 \pm 0.06$ (stat). The total uncertainty on the estimate is $17 \%$, which includes both statistical and systematic uncertainties, which are described in Section 5.

In the $H+1$-jet and $H+2$-jet analyses, the top quark background prediction is normalised to the data in a control sample defined by reversing the $b$-jet veto and removing the requirements on $\Delta \phi_{\ell \ell}$ and $m_{\ell \ell}$. Note that the $\left|\Delta y_{\mathrm{jj}}\right|$ and $m_{\mathrm{jj}}$ requirements are included in the definition of the 2-jet control region. The resulting samples are primarily top events, and the small contribution from other sources is accounted for using simulation and the data-driven $W+$ jets estimate. The predicted and observed dilepton transverse mass distributions of events in these samples are shown in Fig. 4. In these plots, a modified 2 -jet control region, consisting of all events with two or more jets of which at least one is tagged, is used because there are not enough events in the full control region for a meaningful comparison of event kinematics. Good agreement is observed between data and MC for the numbers of events in the $H+1$-jet and $H+2$-jet control regions (see Table 2). The resulting normalisation factors are $1.11 \pm 0.05$ (stat) for the $H+1$-jet analysis and $1.01 \pm 0.26$ (stat) for the $H+2$-jet analysis. The total uncertainties on the estimated top-quark background in the $H+1$-jet and $H+2$-jet signal regions, including both statistical and systematic effects (which are described in Section 5), are 36\% and $70 \%$, respectively.

## 4.3 $W W$ control sample

The $W W$ background MC predictions in the $H+0$-jet and $H+1$-jet analyses, summed over lepton flavours, are normalised using control regions defined with the same selection as the signal region except that the $\Delta \phi_{\ell \ell}$ requirement is removed and the upper bound on $m_{\ell \ell}$ is replaced with a lower bound, $m_{\ell \ell}>80 \mathrm{GeV}$. The numbers of events in the $W W$ control regions in the data agree well with the MC predictions, as can be seen in Table 2. Figure 5 shows the $m_{T}$ shape predicted and observed for events in the $W W$ control regions. Events from $W W$ contribute about $70 \%$ of the total events in the zero jet control region and about $45 \%$ for the one jet control region. Good agreement


Figure 4: Distributions of the $m_{\mathrm{T}}$ variable in the $H+1$-jet (left) $H+2$-jet (right) top control regions. The lepton flavours are combined. The negligible signal shown is for $m_{H}=125 \mathrm{GeV}$. The $H+1$-jet top control region is identical to the $H+1$-jet signal region except that the veto on a $b$-tagged jet is reversed. The $H+2$-jet top control region used here is defined by the requirement of two or more jets, one of which is $b$-tagged jet, after the dilepton and $E_{\mathrm{T}, \text { rel }}^{\text {miss }}$ preselection. It is larger than but contains the sample used to normalise the top background in the $H+2$-jet analysis. No data-driven normalisation factors are applied to the simulated data. The hashed area indicates the total uncertainty on the background prediction.
is observed between the predicted and observed distributions. Contributions from sources other than $W W$ are derived as they are for the signal region, including the top and $W+$ jets backgrounds. The resulting $W W$ normalisation factors are $1.06 \pm 0.06$ (stat) for the $H+0$-jet channel and $0.99 \pm 0.15$ (stat) for the $H+1$-jet channel. The total uncertainty on the predicted $W W$ background in the signal region, including both statistical and systematic effects (which are described in Section 5), is 13\% for the $H+0$-jet analysis and $42 \%$ for the $H+1$-jet analysis. For the $H+2$-jet analysis, a signaldepleted region with a sufficient number of $W W$ events to make a statistically accurate estimate of this background cannot be isolated and it is therefore predicted using simulation alone.

## 5 Systematic uncertainties

Theoretical uncertainties on the signal production cross sections are determined following Refs. [12, 68]. QCD factorisation and renormalisation scales are independently varied up and down by a factor of two. Independent uncertainties on the ggF signal production are assumed for the inclusive cross section and the cross section for production with at least one or two jets. The resulting uncertainties on the cross sections in exclusive jet multiplicity final states are taken into account, as well as anticorrelations caused by migrations between different jet multiplicities. The sum in quadrature of those uncertainties for $m_{H}=125 \mathrm{GeV}$ amounts to $17 \%$ for the $H+0$-jet, and $36 \%$ for $H+1$-jet, final states $[12,68,69]$. The impact of the scale variations on both the VBF signal cross section and the jet veto acceptance, to which the $H+2$-jet analysis is mainly sensitive, is $4 \%$ [12]. Additional $7 \%$ uncertainties are included to account for the effect of the underlying event modelling on the signal acceptance for VBF signal events after jet tagging and central jet veto cuts. In the $H+2$-jet analysis, approximately $25 \%$ of the signal events are produced via $g g F$, with a relative uncertainty of around 25\%.

PDF uncertainties are evaluated, following Refs. [39, 55, 70, 71], using the envelopes of error sets


Figure 5: $m_{T}$ distributions in the $W W$ control region in the $H+0$-jet (left) and $H+1$-jet (right) analyses. The lepton flavours are combined. The signal shown is for $m_{H}=125 \mathrm{GeV}$. The top backgrounds are scaled using the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.
as well as different PDF sets, applied separately to quark-quark, quark-gluon, and gluon-gluon initiated processes. For $m_{H}=125 \mathrm{GeV}$ the relative PDF uncertainty is $8 \%$ for the ggF process and $2 \%$ for the VBF process. Uncertainties on the modelling of signal processes are estimated by using alternative generators, such as MC@NLO for the acceptance for the ggF process. As described in Section 4, the $W W$ background is normalised to signal-free control regions. The theoretical uncertainty on the extrapolation to the signal region from the control regions has been evaluated according to the prescription of [12]. An additional modelling uncertainty is added to take into account differences in the number of extrapolated events obtained with MC@NLO+HERWIG and POWHEG+PYTHIA8. The uncertainties associated with the underlying event and parton showering are included in the acceptance uncertainty, although they are negligible compared to the scale uncertainties on the cross sections for $H+0$-jet and $H+1$-jet.

Uncertainties on the $W \gamma$ background normalisation are evaluated for each jet bin using the procedure described in [68]. The uncertainty relative to the predicted $W \gamma$ background is $11 \%$ for the 0 -jet bin and $50 \%$ for the 1 -jet bin. For $W \gamma^{*}$ with $m_{\ell \ell}<7 \mathrm{GeV}$, a K-factor of $1.3 \pm 0.3$ is applied to the MadGraph LO prediction based on the comparison with the MCFM NLO calculation. The corresponding K-factor and uncertainty for $W Z^{(*)}$ with $m_{\ell \ell}>7 \mathrm{GeV}$ is $1.51 \pm 0.45$.

The main experimental uncertainties are related to the jet energy scale, which is determined from a combination of test beam, simulation, and in situ measurements. The uncertainty on the jet energy scale varies from $2 \%$ to $9 \%$ as a function of jet $p_{\mathrm{T}}$ and $\eta$ for jets with $p_{\mathrm{T}}>25 \mathrm{GeV}$ and $|\eta|<4.5$ [72]. An additional contribution to the jet energy scale uncertainty arises from pile-up, and is is estimated to vary between $1 \%$ and $5 \%$ for in-time pile-up, and up to $10 \%$ for out-of-time pile-up. The jet energy resolution varies from $7 \%$ to $22 \%$ as a function of jet $p_{\mathrm{T}}$ and $\eta$, and the relative systematic uncertainty on it, determined from in situ measurements, ranges from $17 \%$ to $25 \%$. The reconstruction, identification, and trigger efficiencies for electrons and muons, as well as their momentum scales and resolutions, are estimated using $Z \rightarrow \ell \ell, J / \psi \rightarrow \ell \ell$, and $W \rightarrow \ell v$ decays $(\ell=e, \mu)$. With the exception of the uncertainty on the electron selection efficiency, which varies between $2 \%$ and $5 \%$ as a function of $p_{\mathrm{T}}$ and $\eta$, the resulting uncertainties are all smaller than $1 \%$. Jet energy scale and lepton momentum scale uncertainties are propagated to the $E_{\mathrm{T}}^{\text {miss }}$ computation. Additional contributions arise from jets with $p_{\mathrm{T}}<20 \mathrm{GeV}$ as well as from low-energy calorimeter deposits not associated with reconstructed physics objects [61]; their effect on the total signal and background yields is about 3\%. The efficiency
of the $b$-tagging algorithm is calibrated using samples containing muons reconstructed in the vicinity of jets [64]. The resulting uncertainty on the $b$-jet tagging efficiency varies between $5 \%$ and $18 \%$ as a function of jet $p_{\mathrm{T}}$. The preliminary uncertainty on the integrated luminosity is $3.6 \%$, based on the calibration described in Ref. [73, 74].

For the backgrounds normalised using control regions, the systematic uncertainties are evaluated on the relative normalisation between the backgrounds in the signal and control regions and on the $m_{\mathrm{T}}$ shape in the signal region. The uncertainty on the top background in the $H+0$-jet analysis is dominated by the size of neglected interference effects between $t \bar{t}$ and single top and by the impact of the choice of jet thresholds on top event kinematics. Systematic uncertainties are evaluated for the control regions described in Section 4 in the same way as for the signal regions.

In this analysis, a fit to the $m_{\mathrm{T}}$ distribution is performed in order to obtain the signal yield for each mass hypothesis. The $m_{\mathrm{T}}$ shapes for the individual backgrounds and signal do not exhibit a statistically significant dependence on the majority of the theoretical and experimental uncertainties. The remaining uncertainties that do produce statistically significant variations of the $m_{\mathrm{T}}$ shape have no appreciable effect on the final results, with the exception of the $W W$ background, where an uncertainty is included to take into account differences in the $m_{T}$ shape observed between the MC@NLO and POWHEG generators. However, the uncertainty on the shape of the total background is dominated by the uncertainties on the normalisations of the individual backgrounds.

## 6 Results

### 6.1 Results from the 8 TeV data

The expected numbers of signal ( $m_{H}=125 \mathrm{GeV}$ ) and background events at several stages of the selection are presented in Table 2. The rightmost column shows the observed numbers of events in the data. The uncertainties shown include only the statistical uncertainties on the predictions from simulation. After all selection criteria, the dominant background in the $H+0$-jet channel comes from continuum $W W$ production, with smaller contributions from top, non- $W W$ diboson, and $W+$ jets events. In the $H+1$-jet and $H+2$-jet channels, the $W W$ and top backgrounds are comparable. Figure 6 shows the distributions of the transverse mass after all selection criteria in the $H+0$-jet and $H+1$-jet analyses, for both lepton channels combined. No distributions are shown for the $H+2$-jet channel because only two events in the data pass all of the selection through the $\Delta \phi_{\ell \ell}$ requirement.

Figure 7 shows the transverse mass distributions in data after all selection criteria have been applied, with the total estimated background subtracted. The $H+0$-jet and $H+1$-jet channels are summed and the predicted $m_{H}=125 \mathrm{GeV}$ signal is superimposed. No systematic uncertainties are included.

Table 3 shows the numbers of events expected from signal and background and observed in data, after application of all selection criteria. To reflect better the sensitivity of the analysis, additional thresholds on $m_{\mathrm{T}}$ have been applied: $0.75 m_{H}<m_{\mathrm{T}}<m_{H}$ for $m_{H}=125 \mathrm{GeV}$. The results are shown for the $e \mu$ and $\mu e$ channels combined. The uncertainties shown in Table 3 include the systematic uncertainties discussed in Section 5, constrained by the use of the control regions discussed in Section 4. The uncertainties are those that enter into the fitting procedure described below. An excess of events relative to the predicted background is observed in the data. Table 4 shows the magnitude of the main sources of systematic uncertainty on the signal ( $m_{H}=125 \mathrm{GeV}$ ) and background predictions for the $H+0$-jet and $H+1$-jet analyses. Similarly to Table 3 , the additional $m_{\mathrm{T}}$ cut is applied and the constraints from control regions are included.

The statistical analysis of the data employs a binned likelihood function $\mathcal{L}(\mu, \boldsymbol{\theta})$ constructed as the product of Poisson probability terms in each lepton flavour channel. The $m_{H}$-dependent $m_{\mathrm{T}}$ thresholds

Table 2: The expected numbers of signal and background events after the requirements listed in the first column, as well as the observed numbers of events. The signal is shown for $m_{H}=125 \mathrm{GeV}$. The $W+$ jets background is estimated entirely from data, whereas MC predictions normalised to data in control regions are used for the $W W, t \bar{t}$, and $t W / t b / t q b$ processes in all the stages of the selection. Contributions from other background sources are taken entirely from MC predictions. The expected numbers of signal and background events, and the observed numbers of events, are shown also in the control regions. For these rows, the $W+$ jets contribution is still taken from the data-driven estimate but no normalisation factors are applied, except that the top normalisation factor is applied for the top background estimate in the $W W$ control regions. The bottom part of the table lists the number of expected and observed events after the $\Delta \phi_{\ell \ell}$ cut separated by the flavour of the subleading lepton. Only statistical uncertainties associated with the number of events in the MC samples are shown.

| Cutflow evolution in the different signal regions |  |  |  |  |  |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $H+0$-jet | Signal | $W W$ | $W Z / Z Z / W \gamma$ | $t \bar{t}$ | $t W / t b / t q b$ | $Z / \gamma^{*}+$ jets | $W+$ jets | Total Bkg. | Obs. |
| Jet Veto | $47.5 \pm 0.4$ | $1308 \pm 9$ | $125 \pm 4$ | $184 \pm 4$ | $109 \pm 6$ | $850 \pm 32$ | $138 \pm 4$ | $2714 \pm 34$ | 2691 |
| $p_{\mathrm{T}}^{\ell \ell}>30 \mathrm{GeV}$ | $43.4 \pm 0.4$ | $1077 \pm 8$ | $99 \pm 4$ | $165 \pm 4$ | $98 \pm 5$ | $47 \pm 8$ | $102 \pm 2$ | $1589 \pm 14$ | 1664 |
| $m_{\ell \ell}<50 \mathrm{GeV}$ | $34.9 \pm 0.4$ | $244 \pm 4$ | $33 \pm 2$ | $28 \pm 2$ | $17 \pm 2$ | $5 \pm 2$ | $29 \pm 1$ | $356 \pm 6$ | 421 |
| $\Delta \phi_{\ell \ell}<1.8$ | $33.6 \pm 0.4$ | $234 \pm 4$ | $32 \pm 2$ | $27 \pm 2$ | $17 \pm 2$ | $4 \pm 2$ | $25 \pm 1$ | $339 \pm 6$ | 407 |
| $H+1$-jet | Signal | $W W$ | $W Z / Z Z / W \gamma$ | $t \bar{t}$ | $t W / t b / t q b$ | $Z / \gamma^{*}+$ jets | $W+$ jets | Total Bkg. | Obs. |
| 1 jet | $24.9 \pm 0.3$ | $396 \pm 5$ | $74 \pm 3$ | $1652 \pm 12$ | $479 \pm 12$ | $283 \pm 20$ | $68 \pm 3$ | $2953 \pm 27$ | 2874 |
| $b$-jet veto | $21.1 \pm 0.3$ | $334 \pm 4$ | $56 \pm 2$ | $349 \pm 6$ | $115 \pm 6$ | $236 \pm 18$ | $53 \pm 2$ | $1144 \pm 21$ | 1115 |
| $\left\|\mathbf{p}_{\mathrm{T}}^{\text {tot }}\right\|<30 \mathrm{GeV}$ | $12.2 \pm 0.2$ | $210 \pm 3$ | $30 \pm 2$ | $139 \pm 4$ | $63 \pm 5$ | $124 \pm 14$ | $23 \pm 2$ | $590 \pm 15$ | 611 |
| $Z \rightarrow \tau \tau$ veto | $12.2 \pm 0.2$ | $204 \pm 3$ | $29 \pm 2$ | $133 \pm 3$ | $61 \pm 5$ | $98 \pm 12$ | $23 \pm 2$ | $547 \pm 14$ | 580 |
| $m_{\ell \ell}<50 \mathrm{GeV}$ | $9.2 \pm 0.2$ | $37 \pm 1$ | $10 \pm 1$ | $21 \pm 1$ | $12 \pm 2$ | $16 \pm 5$ | $8.0 \pm 0.9$ | $104 \pm 6$ | 122 |
| $\Delta \phi_{\ell \ell}<1.8$ | $8.6 \pm 0.2$ | $34 \pm 1$ | $9 \pm 1$ | $20 \pm 1$ | $11 \pm 2$ | $3 \pm 2$ | $6.4 \pm 0.7$ | $84 \pm 4$ | 106 |
| $H+2$-jet | Signal | $W W$ | $W Z / Z Z / W \gamma$ | $t \bar{t}$ | $t W / t b / t q b$ | $Z / \gamma^{*}+$ jets | $W+$ jets | Total Bkg. | Obs. |
| $\geq 2$ jets | $14.5 \pm 0.2$ | $139 \pm 3$ | $30 \pm 2$ | $7039 \pm 24$ | $376 \pm 11$ | $104 \pm 12$ | $71 \pm 4$ | $7759 \pm 29$ | 7845 |
| $b$-jet veto | $9.6 \pm 0.2$ | $95 \pm 2$ | $19 \pm 1$ | $356 \pm 6$ | $44 \pm 4$ | $62 \pm 9$ | $21 \pm 2$ | $597 \pm 12$ | 667 |
| $\left\|\Delta Y_{\mathrm{jj}}\right\|>3.8$ | $2.0 \pm 0.1$ | $8.3 \pm 0.6$ | $2.0 \pm 0.4$ | $31 \pm 2$ | $5 \pm 1$ | $4 \pm 2$ | $1.4 \pm 0.5$ | $52 \pm 3$ | 44 |
| Central jet veto $(20 \mathrm{GeV})$ | $1.6 \pm 0.1$ | $6.5 \pm 0.5$ | $1.3 \pm 0.3$ | $16 \pm 1$ | $4 \pm 1$ | $1 \pm 1$ | $0.5 \pm 0.3$ | $29 \pm 2$ | 22 |
| $m_{\mathrm{jj}}>500 \mathrm{GeV}$ | $1.1 \pm 0.0$ | $3.2 \pm 0.4$ | $0.7 \pm 0.2$ | $6.2 \pm 0.7$ | $1.8 \pm 0.6$ | $0.0 \pm 0.0$ | $0.0 \pm 0.2$ | $12 \pm 1$ | 13 |
| $\left\|\mathbf{p}_{\mathrm{T}}^{\text {tot }}\right\|<30 \mathrm{GeV}$ | $0.8 \pm 0.0$ | $1.7 \pm 0.3$ | $0.3 \pm 0.1$ | $2.5 \pm 0.5$ | $0.8 \pm 0.4$ | $0.0 \pm 0.0$ | $0.0 \pm 0.2$ | $5.4 \pm 0.7$ | 6 |
| $Z \rightarrow \tau \tau$ veto | $0.7 \pm 0.0$ | $1.8 \pm 0.3$ | $0.3 \pm 0.1$ | $2.4 \pm 0.4$ | $0.8 \pm 0.4$ | $0.0 \pm 0.0$ | $0.0 \pm 0.2$ | $5.2 \pm 0.7$ | 6 |
| $m_{\ell \ell}<80 \mathrm{GeV}$ | $0.7 \pm 0.0$ | $0.6 \pm 0.2$ | $0.1 \pm 0.1$ | $0.8 \pm 0.3$ | $0.3 \pm 0.2$ | $0.0 \pm 0.0$ | $0.0 \pm 0.2$ | $1.9 \pm 0.5$ | 3 |
| $\Delta \phi_{\ell \ell}<1.8$ | $0.6 \pm 0.0$ | $0.5 \pm 0.2$ | $0.1 \pm 0.1$ | $0.5 \pm 0.3$ | $0.3 \pm 0.2$ | $0.0 \pm 0.0$ | $0.0 \pm 0.2$ | $1.4 \pm 0.4$ | 2 |


| Composition of main control regions |  |  |  |  |  |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Signal | $W W$ | $W Z / Z Z / W \gamma$ | $t \bar{t}$ | $t W / t b / t q b$ | $Z / \gamma^{*}+$ jets | $W+$ jets | Total Bkg. | Obs. |
| $W W$ 0-jet | $0.3 \pm 0.0$ | $531 \pm 5$ | $43 \pm 2$ | $104 \pm 3$ | $62 \pm 4$ | $11 \pm 4$ | $38 \pm 1$ | $789 \pm 9$ | 820 |
| $W W$ 1-jet | $0.1 \pm 0.0$ | $112 \pm 3$ | $13 \pm 1$ | $80 \pm 3$ | $34 \pm 3$ | $9 \pm 4$ | $7.7 \pm 0.8$ | $256 \pm 6$ | 255 |
| Top 1-jet | $2.2 \pm 0.1$ | $39 \pm 2$ | $10 \pm 1$ | $489 \pm 6$ | $195 \pm 7$ | $28 \pm 7$ | $7 \pm 1$ | $768 \pm 12$ | 840 |
| Top 2-jet | $4.9 \pm 0.1$ | $45 \pm 2$ | $11.7 \pm 1.0$ | $6371 \pm 23$ | $315 \pm 10$ | $45 \pm 8$ | $52 \pm 3$ | $6840 \pm 26$ | 7178 |


| Signal region yield for $e \mu$ and $\mu e$ channels separately |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: |
|  | 0 -jet $e \mu$ | 0 -jet $\mu e$ | 1 -jet $e \mu$ | 1 -jet $\mu e$ |
| Total bkg. | $177 \pm 4$ | $162 \pm 4$ | $43 \pm 2$ | $40 \pm 3$ |
| Signal | $18.7 \pm 0.3$ | $14.9 \pm 0.2$ | $4.3 \pm 0.1$ | $4.2 \pm 0.1$ |
| Observed | 213 | 194 | 54 | 52 |



Figure 6: Transverse mass, $m_{\mathrm{T}}$, distribution in the $H+0$-jet (top) and $H+1$-jet (bottom) channels, for events satisfying all criteria. The plots on the left show the events with a subleading muon, and the plots on the right show the events with a subleading electron. The expected signal for a SM Higgs boson with $m_{H}=125 \mathrm{GeV}$ is added on top of the estimated total background. The $W+$ jets background is estimated directly from data and $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.

Table 3: The expected numbers of signal ( $m_{H}=125 \mathrm{GeV}$ ) and background events after the full selections, including a cut on the transverse mass of $0.75 m_{H}<m_{\mathrm{T}}<m_{H}$ for $m_{H}=125 \mathrm{GeV}$. The observed numbers of events are also displayed. The uncertainties shown are the combination of the statistical and all systematic uncertainties, taking into account the constraints from control samples. These results differ from those given in Table 2 due to the application of the additional $m_{\mathrm{T}}$ cut. All numbers are summed over lepton flavours. For the $H+2$-jet analysis, backgrounds with fewer than 0.01 events expected are marked as negligible using a '-'.

|  | Signal | $W W$ | $W Z / Z Z / W \gamma$ | $t \bar{t}$ | $t W / t b / t q b$ | $Z / \gamma^{*}+$ jets | $W+$ jets | Total Bkg. | Obs. |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $H+0$-jet | $20 \pm 4$ | $101 \pm 13$ | $12 \pm 3$ | $8 \pm 2$ | $3.4 \pm 1.5$ | $1.9 \pm 1.3$ | $15 \pm 7$ | $142 \pm 16$ | 185 |
| $H+1$-jet | $5 \pm 2$ | $12 \pm 5$ | $1.9 \pm 1.1$ | $6 \pm 2$ | $3.7 \pm 1.6$ | $0.1 \pm 0.1$ | $2 \pm 1$ | $26 \pm 6$ | 38 |
| $H+2$-jet | $0.34 \pm 0.07$ | $0.10 \pm 0.14$ | $0.10 \pm 0.10$ | $0.15 \pm 0.10$ | - | - | - | $0.35 \pm 0.18$ | 0 |

described above are not used. Instead, the $m_{\mathrm{T}}$ distribution of events satisfying all of the criteria up to and including the $\Delta \phi_{\ell \ell}$ requirement is fit using the binned likelihood, with the $H+0$-jet $(H+$


Figure 7: The $m_{\mathrm{T}}$ distribution in data with the estimated background subtracted, overlaid with the predicted signal for $m_{H}=125 \mathrm{GeV}$. The distributions are summed for the $H+0$-jet and $H+1$-jet analyses. The statistical errors of both the data and the subtracted background are reflected in the data points. The systematic uncertainty on the background estimate is not included.

1-jet) signal regions subdivided into five (three) $m_{\mathrm{T}}$ bins. For the $H+2$-jet signal region, and the $W W$ and top control regions, only the results integrated over $m_{\mathrm{T}}$ are used; no shape information is used due to the small number of events remaining after the event selection. The use of the $m_{T}$ fit in place of a selection of events in a range of $m_{T}$ increases the sensitivity of the analysis but also incurs additional systematic uncertainties on the modelling of the shape of the $m_{T}$ distribution for the backgrounds. These additional uncertainties are not included in Table 3, but they are small in comparison to the uncertainties on the normalisation. The potential impact of the interference between $W W$ and Higgs diagrams [75] above a value of $m_{T}$ corresponding to the Higgs mass was investigated and found to be negligible. A "signal strength" parameter $\mu$ multiplies the expected Standard Model Higgs boson production signal in each bin. Signal and background predictions depend on systematic uncertainties that are parametrised by nuisance parameters $\boldsymbol{\theta}$, which in turn are constrained using Gaussian functions. The expected signal and background event counts in each bin are functions of $\boldsymbol{\theta}$. The parametrisation is chosen such that the rates in each channel are log-normally distributed for a normally distributed $\theta$. The test statistic $q_{\mu}$ is then constructed using the profile likelihood: $q_{\mu}=-2 \ln \left(\mathcal{L}\left(\mu, \hat{\boldsymbol{\theta}}_{\mu}\right) / \mathcal{L}(\hat{\mu}, \hat{\boldsymbol{\theta}})\right)$, where $\hat{\mu}$ and $\hat{\boldsymbol{\theta}}$ are the parameters that maximise the likelihood (with the constraint $0 \leq \hat{\mu} \leq \mu$ ), and $\hat{\boldsymbol{\theta}}_{\mu}$ are the nuisance parameter values that maximise the likelihood for a given $\mu$. This test statistic is used to compute the probability $\left(p_{0}\right)$ that a background fluctuation is more signal-like than the observed data, and to calculate the exclusion limits following the modified frequentist method known as $C L_{s}[76,77]$.

Figure 8 shows the expected and observed $p_{0}$ value and the fitted signal strength $\mu$ over the range $110<m_{H}<190 \mathrm{GeV}$, for the combined $H+0$-jet, $H+1$-jet and $H+2$-jet analyses. An excess of events is observed over the expected background, reflected by a low observed $p_{0}$ and a fitted $\mu$ which deviates from zero. Due to the limited mass resolution for this analysis, the $p_{0}$ distribution is rather flat around $m_{H}=125 \mathrm{GeV}$. The value of $p_{0}$ at $m_{H}=125 \mathrm{GeV}$ is $8 \times 10^{-4}$, corresponding to 3.1 standard deviations. The minimum value of $p_{0}$, found at $m_{H}=120 \mathrm{GeV}$, is $6 \times 10^{-4}$, which corresponds to 3.2 standard deviations. The significance exceeds three standard deviations for a possible signal within the mass range $110-130 \mathrm{GeV}$. The expected $p_{0}$ for a Higgs with $m_{H}=125 \mathrm{GeV}$ is 0.05

Table 4: Main systematic uncertainties on the predicted numbers of signal ( $m_{H}=125 \mathrm{GeV}$ ) and background events for the $H+0$-jet and $H+1$-jet analyses, relative to the total signal and background expectations. The same $m_{\mathrm{T}}$ criteria as in Table 3 are imposed. All numbers are summed over lepton flavours. The effect of the quoted inclusive signal cross section renormalisation and factorisation scale uncertainties on exclusive jet multiplicities is explained in Section 5. Sources of uncertainty that are negligible or not applicable in a particular column are marked with a '-'.

| Source (0-jet) | Signal (\%) | Bkg. (\%) |
| :--- | ---: | ---: |
| Inclusive ggF signal ren./fact. scale | 13 | - |
| 1-jet incl. ggF signal ren./fact. scale | 10 | - |
| Parton distribution functions | 8 | 2 |
| Jet energy scale | 7 | 4 |
| $W W$ normalisation | - | 7 |
| $W W$ modelling and shape | - | 5 |
| $W+$ +jets fake factor | - | 5 |
| QCD scale acceptance | 4 | 2 |
| Source (1-jet) | Signal (\%) | Bkg. (\%) |
| 1-jet incl. ggF signal ren./fact. scale | 28 | - |
| WW normalisation | 0 | 25 |
| 2-jet incl. ggF signal ren./fact. scale | 16 | - |
| $b$-tagging efficiency | - | 10 |
| Parton distribution functions | 7 | 1 |
| $W+$ +jets fake factor | 0 | 5 |

or 1.6 standard deviations. The fitted signal strength is also shown in Figure 8 and is $\mu=1.9 \pm 0.7$ at $m_{H}=126 \mathrm{GeV}$, the location of the minimum observed $p_{0}$ in the most recent ATLAS combined results [78]. The increase of the fitted signal strength at lower $m_{H}$ is due to the decreasing expected $\sigma \cdot B r$ for the signal.

As a comparison, the $p_{0}$ was also evaluated using a counting experiment after applying a requirement on $0.75 m_{H}<m_{\mathrm{T}}<m_{H}$, rather than fitting the $m_{T}$ distribution (see Table 3 for event yields after the requirement on $m_{T}$ has been applied for $m_{H}=125 \mathrm{GeV}$ ). The resulting decrease in sensitivity reduces the expected significance at $m_{H}=125 \mathrm{GeV}$ to $p_{0}=0.07$ or 1.5 standard deviations. The observed significance in this variant of the analysis reaches a minimum of $p_{0}=2 \times 10^{-3}$, equivalent to 3.0 standard deviations, at $m_{H}=125 \mathrm{GeV}$.

The expected $95 \% C L_{S}$ limit on $\sigma / \sigma_{S M}$ excludes a SM Higgs boson with a mass down to 129 GeV . However, due to the observed excess of events the observed excluded $C L_{s}$ lower limit is only at 145 GeV .

### 6.2 Combination of the 7 TeV and 8 TeV results

The results obtained with the $5.8 \mathrm{fb}^{-1}$ of 8 TeV data acquired in 2012 are combined with the published $4.7 \mathrm{fb}^{-1}$ of 7 TeV results [13]. The 7 TeV analysis resulted in a signal strength of $\mu=0.5 \pm 0.6$ at $m_{H}=126 \mathrm{GeV}$. The signal strengths measured with the 7 TeV and 8 TeV analyses separately are compatible within 1.5 standard deviations. Figure 9 shows the distribution of the transverse mass after all selection criteria have been applied, summed for the 7 TeV and 8 TeV data, after subtracting the total estimated background. The $H+0$-jet and $H+1$-jet channels are added and the predicted $m_{H}=125 \mathrm{GeV}$ signal is superimposed. No systematic uncertainties are included. This figure is the equivalent of Figure 7 for the combined 2011 and 2012 datasets.

Figure 10 shows the expected and observed $p_{0}$ value and the fitted signal strength for the $H+0$-jet,


Figure 8: 2012 results, using $5.8 \mathrm{fb}^{-1}$ of 8 TeV data. Left: observed (solid line) probability for the background-only scenario as a function of $m_{H}$. The dashed line shows the corresponding expectation for the signal+background hypothesis at the given value of $m_{H}$. Right: fitted signal strength parameter $(\mu)$ as a function of $m_{H}$ for the low mass range.
$H+1$-jet and $H+2$-jet analyses with 7 TeV and 8 TeV data combined. Also shown is the expected distribution in the presence of a Higgs boson with $m_{H}=125 \mathrm{GeV}$. An excess of events is observed over the expected background, reflected by a low observed $p_{0}$ and a fitted $\mu$ which deviates from zero. The minimum value observed for $p_{0}$, found at $m_{H}=125 \mathrm{GeV}$, is $3 \times 10^{-3}$, corresponding to 2.8 standard deviations. The expected $p_{0}$ for a Higgs with $m_{H}=125 \mathrm{GeV}$ is 0.01 , or 2.3 standard deviations, for the combined 7 TeV and 8 TeV data. The fitted signal strength at $m_{H}=126 \mathrm{GeV}$ is $\mu$ $=1.3 \pm 0.5$.

Figure 11 shows the two-dimensional likelihood contours for a simultaneous scan of $\mu$ and $m_{H}$, for this analysis and also for the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ [79] and $H \rightarrow \gamma \gamma$ [80] analyses. The lack of mass resolution in the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell v$ final state for low $m_{H}$ can be seen clearly in contrast to the $H \rightarrow Z Z^{(*)} \rightarrow 4 \ell$ and $H \rightarrow \gamma \gamma$ final states, but the best-fit values of $\mu$ and $m_{H}$ are in reasonable agreement for all three analyses.

Figure 12 shows the observed local $p_{0}$ from the combined 7 TeV and 8 TeV results, compared to the one expected in the presence of a signal at $m_{H}=125 \mathrm{GeV}$. The shape and normalisation of the $p_{0}$ curves as a function of $m_{H}$ are in agreement.

The $95 \% C L_{s}$ limit on $\sigma / \sigma_{S M}$ is expected to exclude a SM Higgs boson with a mass above 124 GeV with the combined 7 TeV and 8 TeV data in the absence of a signal. However, due to the observed excess of events the observed exclusion $C L_{s}$ lower limit is found at 137 GeV . The $C L_{s}$ limit is shown in Figure 12.

## 7 Conclusion

A search for the SM Higgs boson has been performed in the $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell v$ channel in the mass range between 110 and 190 GeV using a data sample corresponding to $5.8 \mathrm{fb}^{-1}$ of $p p$ collision data from the Large Hadron Collider at $\sqrt{s}=8 \mathrm{TeV}$ recorded in 2012 with the ATLAS detector. For $m_{H} \lesssim 150 \mathrm{GeV}$, an excess of events over the expected background is observed, with a minimum local $p_{0}$-value of $6 \times 10^{-4}$ at $m_{H}=120 \mathrm{GeV}$, or 3.2 standard deviations. A combined analysis of the 2011 and 2012 data results in a minimum local $p_{0}$ at $m_{H}=125 \mathrm{GeV}$ of $3 \times 10^{-3}$, or 2.8 standard deviations. The best fit signal strength at $m_{H}=126 \mathrm{GeV}$, the location of the minimum observed $p_{0}$ in the most recent ATLAS combined results [78], cross section, is $1.3 \pm 0.5$. Given the observation of a new boson


Figure 9: The $m_{\mathrm{T}}$ distribution in data with the estimated background subtracted, overlaid with the predicted signal for $m_{H}=125 \mathrm{GeV}$. The distributions are summed for the $H+0$-jet and $H+1$-jet analyses and the 7 TeV and 8 TeV data. The statistical errors of both the data and the subtracted background are reflected in the data points. The systematic uncertainty on the background estimate is not included.


Figure 10: Combined 7 TeV and 8 TeV results. Left: observed (solid line) probability for the background-only scenario as a function of $m_{H}$. The dashed line shows the corresponding expectation for the signal+background hypothesis at the given value of $m_{H}$. Right: fitted signal strength parameter $(\mu)$ as a function of $m_{H}$ for the low mass range (solid black line with cyan band). The expected result for a signal hypothesis of $m_{H}=125 \mathrm{GeV}$ (red line) is included for comparison.
with mass close to 125 GeV in the $Z Z^{(*)}$ and $\gamma \gamma$ final states [79, 80], the excess observed in the $\ell \nu \ell$ final state is consistent with the decay of this new particle into a pair of $W$ bosons.


Figure 11: Approximate $68 \%$ and $95 \%$ two-dimensional likelihood $\left(\lambda\left(\mu, m_{H}\right)\right)$ contours in the best-fit signal strength $\mu$ and $m_{H}$ for the $W W^{(*)} \rightarrow \ell \nu \ell \nu, Z Z^{(*)} \rightarrow 4 \ell$, and $\gamma \gamma$ analyses using the 2011 and 2012 data [81]. The yellow shading shows the $-\ln \lambda\left(\mu, m_{H}\right)$ values for $H \rightarrow W W^{(*)} \rightarrow \ell \nu \ell \nu$.


Figure 12: Left: Observed (solid line) probability for the background-only scenario, $p_{0}$, as a function of $m_{H}$, for the combined 7 TeV and 8 TeV data. The dashed line shows the corresponding expectation for the $m_{H}=125 \mathrm{GeV}$ hypothesis. Right: Observed (solid) and expected (dashed) $95 \%$ CL upper limits on the cross section, normalised to the SM Higgs boson production cross section and as a function of $m_{H}$, over the full mass range considered in the 7 and 8 TeV combined data. Due to the excess of events observed in the low mass signal region, the corresponding mass points cannot be excluded as expected. The results at neighbouring mass points are highly correlated due to the limited mass resolution in this final state. The green and yellow regions indicate the $\pm 1 \sigma$ and $\pm 2 \sigma$ uncertainty bands on the expected $p_{0} /$ limit, respectively.

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## A Additional Figures



Figure 13: Distributions for the same-sign validation region; leading lepton $p_{\mathrm{T}}$ (top left) and subleading lepton $p_{\mathrm{T}}$ (top right) after the zero jet veto and leading lepton $p_{\mathrm{T}}$ (bottom left) and sub-leading lepton $p_{\mathrm{T}}$ (bottom right) after the one jet requirement. The $e \mu$ and $\mu$ e channels are combined. The signal shown is for $m_{H}=125 \mathrm{GeV}$. The hashed area indicates the total uncertainty on the background prediction.


Figure 14: Kinematic distributions in the $H+0$-jet channel. $p_{\mathrm{T}}^{\ell \ell}$ after the zero jet veto (left), and $m_{\ell \ell}$ after the cut on $p_{\mathrm{T}}^{\ell \ell}$ (right). The signal shown is added on top of the background and is for $m_{H}=125 \mathrm{GeV}$. The $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.


Figure 15: Kinematic distributions in the $H+0$-jet channel after full selection $\left(\Delta \phi_{\ell \ell}<1.8\right)$ : $p_{\mathrm{T}}^{\ell \ell}$ (top left), $\Delta \phi_{\ell \ell}$ (top right), $m_{\ell \ell}$ (bottom left), and $m_{\mathrm{T}}$ (bottom right). The $e \mu$ and $\mu$ e channels are combined. The signal shown is added on top of the background and is for $m_{H}=125 \mathrm{GeV}$. The $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.


Figure 16: Kinematic distributions in the $H+0$-jet channel after full selection ( $\Delta \phi_{\ell \ell}<1.8$ ): leading lepton $p_{\mathrm{T}}$ (left) and sub-leading lepton $p_{\mathrm{T}}$ (right). The $e \mu$ and $\mu$ e channels are combined. The signal shown is added on top of the background and is for $m_{H}=125 \mathrm{GeV}$. The $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.


Figure 17: Kinematic distributions in the $H+1$-jet channel. $\left|\mathbf{p}_{\mathrm{T}}^{\text {tot }}\right|$ after the $b$-jet veto (left), and $m_{\ell \ell}$ after the $Z \rightarrow \tau \tau$ veto (right). The signal shown is added on top of the background and is for $m_{H}=125 \mathrm{GeV}$. The $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.


Figure 18: Kinematic distributions in the $H+1$-jet channel after full selection ( $\Delta \phi_{\ell \ell}<1.8$ ): $p_{\mathrm{T}}^{\ell \ell}$ (top left), $\Delta \phi_{\ell \ell}$ (top right), $m_{\ell \ell}$ (bottom left), and $m_{\mathrm{T}}$ (bottom right). The e $\mu$ and $\mu \mathrm{e}$ channels are combined. The signal shown is added on top of the background and is for $m_{H}=125 \mathrm{GeV}$. The $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.



Figure 19: Kinematic distributions in the $H+1$-jet channel after full selection ( $\Delta \phi_{\ell \ell}<1.8$ ): leading lepton $p_{\mathrm{T}}$ (left) and sub-leading lepton $p_{\mathrm{T}}$ (right). The $e \mu$ and $\mu$ e channels are combined. The signal shown is added on top of the background and is for $m_{H}=125 \mathrm{GeV}$. The $W W$ and top backgrounds are scaled to use the normalisation derived from the corresponding control regions described in the text. The hashed area indicates the total uncertainty on the background prediction.


Figure 20: Observed (solid) and expected (dashed) $95 \%$ CL upper limits on the cross section, normalised to the SM Higgs boson production cross section and as a function of $m_{H}$, over the full mass range considered in the 8 TeV data. The green and yellow regions indicate the $\pm 1 \sigma$ and $\pm 2 \sigma$ uncertainty bands on the expected limit, respectively. Due to the excess of events observed in the low mass signal region, the corresponding mass points cannot be excluded as expected. The results at neighbouring mass points are highly correlated due to the limited mass resolution in this final state.


Figure 21: Display of an event satisfying all the selection criteria for events in the $H+0$-jet $e \mu$ channel. The reconstructed lepton $p_{\mathrm{T}}$ values are 33 and 29 GeV for the electron and the muon respectively. The reconstructed $E_{\mathrm{T}, \text { rel }}^{\mathrm{miss}}$ is 35 GeV and the $m_{\mathrm{T}}$ is 94 GeV . ATLAS NOTE

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# Search for Charged Higgs Bosons in the $\tau+$ jets Final State in $t \bar{t}$ Decays with $1.03 \mathrm{fb}^{-1}$ of $p p$ Collision Data Recorded at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS Experiment 

The ATLAS Collaboration


#### Abstract

This note presents the results of a search for charged Higgs bosons, $H^{ \pm}$, in $1.03 \mathrm{fb}^{-1}$ of proton-proton collision data recorded at $\sqrt{s}=7 \mathrm{TeV}$ with the ATLAS experiment at the LHC using the $\tau+$ jets channel in $t \bar{t}$ decays with a hadronically decaying $\tau$ lepton in the final state. The data agree with the Standard Model expectation leading to a limit on the product of branching ratios $\mathrm{BR}\left(t \rightarrow b H^{ \pm}\right) \times \mathrm{BR}\left(H^{ \pm} \rightarrow \tau v\right)$ of $0.03-0.10$ for $H^{ \pm}$masses in the range $90 \mathrm{GeV}<m_{H^{ \pm}}<160 \mathrm{GeV}$. In the context of the Minimal Supersymmetric Standard Model values of $\tan \beta$ larger than $22-30$ are excluded in the mass range $90 \mathrm{GeV}<m_{H^{ \pm}}<140 \mathrm{GeV}$.


## 1 Introduction

The charged Higgs boson is predicted by many non-minimal Higgs scenarios [1, 2], such as models containing Higgs triplets and Two-Higgs-Doublet Models (2HDM) [3]. The observation of charged Higgs bosons ${ }^{1}, H^{ \pm}$, would indicate physics beyond the Standard Model (SM). The analysis in this note considers the type II-2HDM [3], which is also the Higgs sector of the Minimal Supersymmetric Standard Model (MSSM) [4]. For charged Higgs boson masses, $m_{H^{+}}$, smaller than the top quark mass, $m_{t}$, the dominant production mode at the LHC for $H^{+}$is through top quark decay via $t \rightarrow H^{+} b$. The dominant source of top quarks at the LHC is through $t \bar{t}$ production; the cross section for charged Higgs boson production from top quark decays in single-top events is much smaller and not considered here. For $\tan \beta>3$, where $\tan \beta$ is the ratio of the vacuum expectation values of the two Higgs doublets, charged Higgs bosons decay mainly via $H^{+} \rightarrow \tau v$ [5]. Recent limits on light charged Higgs boson production come from the Tevatron [6], where the observed upper limit on $\operatorname{BR}\left(t \rightarrow H^{+} b\right)$ assuming $\operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)=1$ is 0.17 for $m_{H^{+}}=120 \mathrm{GeV}$. Direct searches at LEP [7] give a lower limit of $m_{H^{+}} \simeq 90 \mathrm{GeV}$ for $\operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)=1$. Preliminary results for charged Higgs boson searches in top quark decays have recently been made public by the CMS experiment [8].

This note describes the search for charged Higgs bosons in $t \bar{t}$ events in the topology shown in Fig. 1, for the case where both the $\tau$ lepton and the $W$ decay hadronically ( $\tau+\mathrm{jets}$ channel).

The $H^{+}$search uses proton-proton collision data collected with the ATLAS experiment [9] at the LHC at a center-of-mass energy of $\sqrt{s}=7 \mathrm{TeV}$ in 2011. The total integrated luminosity amounts to $1.03 \mathrm{fb}^{-1}$.

The background processes that enter these searches include the production of $t \bar{t}$, single-top, $W+$ jets, $Z / \gamma^{*}+$ jets, and multi-jet events where there is either a true $\tau$ lepton, or another object misidentified as a hadronically decaying $\tau$. In this note, all significant backgrounds, i.e. events with correctly identified hadronically decaying $\tau$ leptons (hereafter referred to as $\tau$ jets), or with jets or electrons misreconstructed as $\tau$ jets, are estimated using data-driven methods.


Figure 1: Example for a leading-order Feynman diagram for the production of a charged Higgs boson through gluon fusion in $t \bar{t}$ decays.

## 2 Physics processes and their cross sections

All relevant backgrounds are estimated using data-driven techniques. However, for backgrounds with intrinsic missing transverse energy and objects misidentified as $\tau$ jets, simulation is used to model any aspects not related to the probability of the object to be misidentified as a $\tau$ jet. For backgrounds without

[^71]intrinsic $E_{\mathrm{T}}^{\text {miss }}$ (multi-jet background), simulation is used to subtract the electroweak and $t \bar{t}$ contribution in the control region. Simulation is also used for comparison with the results of the data-driven estimates.

The Monte Carlo (MC) simulation of $t \bar{t}$ and single-top events is based on MC@NLO [10] using HERWIG [11] for the hadronization process and JIMMY [12] for simulating multi-parton interactions. Overlap between $t \bar{t}$ and single-top final states is taken into account [13]. A $t \bar{t}$ production cross section of 165 pb [14] obtained from approximate NNLO calculations [15] is used (both for SM $t \bar{t}$ decays and decays via a charged Higgs boson). The MC@NLO cross sections are used for single-top production. Throughout this note, a top quark mass of 172.5 GeV is assumed.

ALPGEN [16] is used for the generation of $W+$ jets and $Z / \gamma^{*}+$ jets events with up to five partons from the hard matrix element, again together with HERWIG/JIMMY. The ALPGEN cross sections are rescaled by a factor $1.20(W)$ and $1.25\left(Z / \gamma^{*}\right)$ to match NNLO calculations [17]. The $H^{+}$signal events are generated with PYTHIA [18], using TAUOLA [19] for $\tau$ lepton decays and PHOTOS [20] for photon radiation off charged leptons. Event generators are tuned to describe ATLAS data, and the parameter sets AMBT1 [21] and AUET1 [22] are used for this purpose for events hadronized with Pythia, and with HERWIG/JIMMY, respectively.

Table 1: Simulated events used in this study. The $W / Z+$ jets as well as the $s$ - and $t$-channel single-top events are only simulated for decays involving leptons ( $\ell$ denotes $e, \mu$, or $\tau$ ), and the cross section given includes this branching ratio. The NLO+NNLL cross section is used for $t \bar{t}$, NLO for single-top, and NNLO for $W / Z+$ jets. The $H^{+}$sample uses $m_{H^{+}}=130 \mathrm{GeV}, \operatorname{BR}\left(t \rightarrow b H^{+}\right)=0.1$ and $\operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$ is assumed to be 1 .

| Process | Generator | Cross section [pb] |
| :--- | :--- | ---: |
| $t \bar{t}$ with $\geq 1 \ell$ | MC@NLO | 89.4 |
| single-top $(s, t, W t$ channel $)$ | MC@NLO | $21.4,1.41,14.6$ |
| $W \rightarrow \ell v+$ jets | ALPGEN | $3.1 \cdot 10^{4}$ |
| $Z / \gamma^{*} \rightarrow \ell \ell+$ jets | ALPGEN | $3.2 \cdot 10^{3}$ |
| $t \bar{t} \rightarrow b H^{ \pm} b W$ with $H^{ \pm} \rightarrow \tau v$ | PYTHIA | 29.6 |

All events are propagated through a detailed GEANT4 [23, 24] simulation of the ATLAS detector and reconstructed by the same algorithms as the data. Cross sections and simulated event samples are summarized in Table 1.

## 3 Object reconstruction

A description of the ATLAS detector can be found elsewhere [9]. In this section, the criteria used to identify and reconstruct physics objects such as leptons or jets are described.

Data quality: For both the $H^{+}$event selection and the data-driven background estimates, the following requirements are applied [25]: The sub-detectors relevant to the analyses have been operational, the LHC delivered stable beams, and there are no jets in the event consistent with coming from instrumental effects such as coherent noise in the electromagnetic calorimeter, or non-collision backgrounds. To further reject non-collision backgrounds, only events with a reconstructed primary vertex with at least five associated tracks are considered.

Jets: Jets are reconstructed with the anti- $k_{t}$ algorithm [26,27] with a size parameter value of $R=0.4$. The jet finder uses three-dimensional noise-suppressed clusters [28] in the calorimeter, reconstructed at
the electromagnetic (EM) energy scale. Jets are then calibrated to the hadronic energy scale with Monte-Carlo-based correction factors which depend on their transverse momentum ( $p_{\mathrm{T}}$ ) and pseudorapidity $(\eta)$. The jet energy scale uncertainty is estimated to be $(2.5-14) \%$, depending on $p_{\mathrm{T}}$ and $\eta$, with methods described in Ref. [29] but based on a larger data set. Jets considered in this analysis are required to have $p_{\mathrm{T}}>20 \mathrm{GeV}$ and $|\eta|<2.5$.
$\boldsymbol{b}$ jets: To identify jets initiated by $b$ quarks, a combination of a 3D-impact-parameter-based discriminant and a secondary-vertex-tagger [30] with an identification efficiency of about $60 \%$ for $b$ jets with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $t \bar{t}$ events is applied.
$\boldsymbol{\tau}$ jets: For the reconstruction of $\tau$ jets, all anti- $k_{t}$ jets in the calorimeter with $E_{\mathrm{T}}>10 \mathrm{GeV}$ are considered as $\tau$ candidates [31]. A dedicated algorithm is used to reject electrons (called tight electron veto). Only candidates with 1 or 3 associated tracks reconstructed in the inner detector are considered. Hadronic $\tau$ decays are identified using a likelihood quality criterion (corresponding to an efficiency of about $30 \%$ for $\tau$ leptons with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $Z \rightarrow \tau \tau$ events, and a rejection factor of about 100-1000 for quarkand gluon-initiated jets, depending on $p_{\mathrm{T}}, \eta$, and the number of associated tracks). For this analysis, they are required to have a visible $p_{\mathrm{T}}>20 \mathrm{GeV}$ and to be within $|\eta|<2.3$. In some control regions, a loose $\tau$ identification is used instead; this corresponds to an efficiency of $60 \%$, and a jet rejection of about 10 , depending on $p_{\mathrm{T}}$ and $\eta$.

Electrons: Electrons are reconstructed by matching clustered energy deposits in the electromagnetic calorimeter to tracks reconstructed in the inner detector [32]. They are required to meet quality requirements based on the expected shower shape of electrons [33]. Electrons are required to have $E_{\mathrm{T}}>20 \mathrm{GeV}$, and be isolated (defined by requiring less than 3.5 GeV of transverse energy - after corrections for pileup and leakage - in a cone of $\Delta R=0.2$ around the electron ${ }^{2}$, excluding the electron itself). Electrons are required to be in the fiducial volume of the detector, $|\eta|<2.47$. Electrons in the transition region $1.37<|\eta|<1.52$ are excluded.

Muons: Muon candidates are required to have a match of an inner detector track with a track reconstructed in the muon spectrometer [34]. Candidates are required to have $p_{\mathrm{T}}>10 \mathrm{GeV}$ and $|\eta|<2.5$. Only isolated muons are accepted by requiring that in a cone of $\Delta R=0.3$ around the muon (excluding the muon itself), both the energy deposited in the calorimeters and the momentum of all inner detector tracks total less than 4 GeV of transverse energy.

Missing transverse energy, transverse energy sum: The reconstructed missing transverse energy, $E_{\mathrm{T}}^{\text {miss }}$, is based on the energy deposited in the calorimeter and the momentum of tracks identified as associated to muons. Only noise-suppressed clusters of cells are used, and corrections for unclustered cells are applied. The contribution of the calorimeter cells is calibrated differently depending on which object they are associated to. For all jets, the same hadronic calibration scheme as for jet reconstruction is used while electrons are calibrated at the electromagnetic energy scale [35].

The transverse energy sum, $\sum E_{\mathrm{T}}$, is defined as the sum of the transverse energy of all the objects which have been reconstructed as detailed in this section, including missing transverse energy.

[^72]Overlap removal: When candidates selected using the above criteria overlap geometrically with one another (within $\Delta R<0.2$ ), this conflict is resolved by only selecting one candidate in the following order of priority: muon, electron, $\tau$ jet, or jet.

General systematic uncertainties The main detector-related systematic uncertainties are listed in Table 2. These are mostly related to identification efficiencies and the energy/momentum resolution and scale of the physics objects described above. Uncertainties on trigger efficiency, luminosity, cross sections and acceptance are also listed.

To assess the impact of most sources of systematic uncertainty on the result of the analysis, selection cuts for each analysis are re-applied after shifting a particular parameter by its $\pm 1$ standard deviation uncertainty. The luminosity and the trigger uncertainty with respect to the offline efficiency serve directly as scale factors on the event yield.

Table 2: Systematic uncertainties. Uncertainties on the $t \bar{t}$ cross section include variations of the parton density functions (pdf) and of the factorization and renormalisation scale. A scale factor is the ratio of efficiencies in data and simulation, and is here denoted as "SF". The difference in acceptance for $t \bar{t}$ events at LO and NLO is used as systematic uncertainty on the signal acceptance.

| Quantity | Uncertainty |
| :--- | :--- |
| Luminosity [36] | $\pm 3.7 \%$ |
| Jet energy resolution (JER) | $\pm(10-30) \%$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| Jet energy scale (JES) | $\pm(2.5-14) \%$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $E_{\mathrm{T}}^{\text {miss }}$ | Uncertainty due to scale/resolution uncertainties (e.g. JES); |
|  | additional $10 \%$ of pile-up-related uncertainty |
| $b$-tagging efficiency SF unc. | $\pm(0.05-0.15)$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $b$-tagging mistag rate | $\pm(0.16-0.39)$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $b$ jets JES uncertainty | an additional $\pm 2.5 \%$ on top of the standard JES |
| $\tau$ identification efficiency | $\pm(8.5-9.9) \%$, depending on $p_{\mathrm{T}}$ |
| $\tau$ energy scale | $\pm(4.5-6.5) \%$, depending on $p_{\mathrm{T}}, \eta$, number of associated tracks |
| $\tau$ electron mis-id correction factors | $\pm(23-100) \%$, depending on $\eta$; for one-prong only |
| $\tau+E_{\mathrm{T}}^{\text {miss trigger }}$ | $\pm 9 \%$ |
| $e$ reco. efficiency SF | $\pm(0.7-1.8) \%$, depending on $\eta$ |
| $e$ identification efficiency SF | $\pm(2.2-3.8) \%$, depending on $E_{\mathrm{T}}$ and $\eta$ |
| $e$ energy scale | $\pm(0.3-1.8) \%$, depending on $p_{\mathrm{T}}$ and $\eta$ |
| $e$ energy resolution | $\pm(0.5-2.4) \%$ (additional constant term), depending on $p_{\mathrm{T}}$ and $\eta$ |
| $\mu$ reco. efficiency SF | $\pm(0.25-0.55) \%$, depending on the data-taking period |
| $\mu$ momentum scale and resolution | $\pm(0.4-0.7) \%$, depending on $\eta$ |
| Initial/final state radiation modelling | $-16 \% /+19 \%(t \bar{\tau}$ signal and background) |
| Acceptance | $\pm 4 \%$ (background), $\pm 10 \%$ (signal) |
| $t \bar{t}$ cross section | $165_{-9}^{+4}($ scale $)+7($ pdf $)$ pb |

## 4 Event selection

This study describes the search for a charged Higgs boson in the topology

$$
\begin{equation*}
t \bar{t} \rightarrow\left[H^{+} b\right]\left[W^{-} \bar{b}\right] \rightarrow\left[\left(\tau_{h a d}^{+}+v\right) b\right]\left[\left(q \bar{q}^{\prime}\right) \bar{b}\right] \tag{1}
\end{equation*}
$$

where both the $W$ boson and the $\tau$ lepton decay hadronically. This topology has the advantage that the $W$ boson can be fully reconstructed, the $H^{+}$candidate can be reconstructed in the transverse plane, and
the branching ratio of the $W$ boson decay to quarks is larger than that to leptons; but it needs to be distinguished from a large multi-jet background.

The following selection cuts are applied, based on the reconstructed physics objects described in Section 3:

1. Event preselection:
(a) Data quality cuts.
(b) $E_{\mathrm{T}}^{\text {miss }}$ plus tau trigger $[37,38]$, with a threshold of 29 GeV on the $\tau$ object, of 35 GeV on $E_{\mathrm{T}}^{\text {miss }}$, and no muon corrections on $E_{\mathrm{T}}^{\text {miss }}$. The signal efficiency is about $70 \%$, depending on $m_{H^{+}}$.
(c) At least 4 jets (excluding $\tau$ jets) with $p_{\mathrm{T}}>20 \mathrm{GeV}$ and $|\eta|<2.5$.
2. A $\tau$ jet with $p_{\mathrm{T}}^{\tau}>35 \mathrm{GeV}$ within $|\eta|<2.3$ is required. This $\tau$ jet must be matched to the $\tau$ trigger object within $\Delta R<0.1$. Events with a second identified $\tau$ jet with $p_{\mathrm{T}}^{\tau}>20 \mathrm{GeV}$ are vetoed.
3. Events are vetoed if any identified electrons $\left(E_{\mathrm{T}}>20 \mathrm{GeV}\right)$ or muons $\left(p_{\mathrm{T}}>10 \mathrm{GeV}\right)$ are present.
4. The missing transverse energy $E_{\mathrm{T}}^{\mathrm{miss}}$ is required to be larger than 40 GeV .
5. Events with large reconstructed $E_{\mathrm{T}}^{\mathrm{miss}}$ due to the limited resolution of the energy measurement are rejected with a cut on the ratio $\frac{E_{\mathrm{T}}^{\text {miss }}}{0.5 \cdot \sqrt{\sum E_{\mathrm{T}}}}>8 \mathrm{GeV}^{1 / 2}$, using the $\sum E_{\mathrm{T}}$ definition described in Section 3. Considering the minimum $\sum E_{\mathrm{T}}$ required to pass all other selection cuts, this also corresponds to raising the cut on $E_{\mathrm{T}}^{\text {miss }}$ to about 50 GeV .
6. At least one $b$-tagged jet is required.
7. Topologies consistent with a top decay are identified by requiring that the $q q b$ candidate with the highest $p_{\mathrm{T}}^{q q b}$ value must satisfy $m(q q b) \in[120,240] \mathrm{GeV}$.

For events passing the above selection cuts the transverse mass, $m_{\mathrm{T}}$, is defined as

$$
\begin{equation*}
m_{\mathrm{T}}=\sqrt{2 p_{\mathrm{T}}^{\tau} E_{\mathrm{T}}^{\mathrm{miss}}(1-\cos \Delta \phi)} \tag{2}
\end{equation*}
$$

where $\Delta \phi$ is the azimuthal angle between the $\tau$ jet and the missing energy direction. This final discriminating variable is related to the $W$ boson mass in the $W \rightarrow \tau v$ background case, and the $H^{+}$mass for the signal hypothesis.

At the end of the selection cut flow, after applying data-driven methods as detailed in the sections that follow, $37 \pm 7$ background events are expected for $m_{\mathrm{T}}>40 \mathrm{GeV}$. Of those, $21 \pm 5$ events are expected with a correctly identified $\tau$ jet; about 2 events each for the case where an electron or a jet have been misidentified as a hadronically decaying $\tau$ lepton in a $t \bar{t}$ or electroweak background process. The multijet contribution is expected to be $12 \pm 5$ events. A potential signal yield depends on the charged Higgs boson mass and the branching ratio $t \rightarrow b H^{+}$; for example, 70 events are expected for $m_{H^{+}}=130 \mathrm{GeV}$ and $\operatorname{BR}\left(t \rightarrow b H^{+}\right)=0.1$.

## 5 Data-driven background estimation

The main source of background events to charged Higgs boson searches at the LHC are those coming from production processes such as $t \bar{t}$, multi-jet, single top-quark, and $W+$ jets, in this order of relevance. The individual contributions from these backgrounds are determined in a data-driven way. They can
be divided into two categories: backgrounds with intrinsic $E_{\mathrm{T}}^{\text {miss }}$ from $W$ decays, and backgrounds with $E_{\mathrm{T}}^{\text {miss }}$ caused by detector effects (multi-jet events). For the first category, the contribution from events in which electrons or jets are misidentified as $\tau$ jets are predicted using appropriate control samples while events with correctly identified $\tau$ jets are studied with the embedding method. The multi-jet background can be estimated using the shape of its $E_{\mathrm{T}}^{\text {miss }}$ distribution in a suitable control region.

### 5.1 Methods based on measuring misidentification probabilities

The background from events where an electron or a jet is misidentified as a hadronically decaying $\tau$ lepton is estimated in a data-driven procedure from suitable control samples. The probability for an electron or jet to be misidentified as a $\tau$ jet is defined as
misidentification probability $=\frac{\text { number of } \tau \text { candidates passing event selection, } \tau \text { ID and electron veto }}{\text { number of } \tau \text { candidates passing event selection }}$.

### 5.1.1 Electron-to- $\tau$ misidentification probability with a tag-and-probe method

The Method A tag-and-probe method on $Z / \gamma^{*}$ events in collision data is used to measure the misidentification probability of electrons. The result is compared to simulation, and the ratio of the misidentification probability as measured in data to that determined in simulation is called a scale factor. This factor is then used to correct the description of the electron-to- $\tau$ misidentification probability in simulation. The method used is identical to that described in [39] though based on a larger data set. The process $Z / \gamma^{*} \rightarrow e e$ allows the selection of a clean sample of electrons from data. An electron trigger with a threshold on the electron $E_{\mathrm{T}}$ of 20 GeV is used. The tag electron is required to have a $p_{\mathrm{T}}>30 \mathrm{GeV}$ and to be located in the central region $(|\eta|<2.47)$ of the detector (but outside the transition region between the barrel and the end-cap, $1.37<|\eta|<1.52$ ). It must be isolated (the sum of the momenta of tracks in a cone of $\Delta R=0.4$ around the electron is required to be less than $6 \%$ of the electron momentum) and must pass tight electron identification criteria [33]. Furthermore, a match within $\Delta R=0.1$ to the trigger electron is required. The probe electron is considered for further analysis if it is reconstructed as a $\tau$ jet candidate with $p_{\mathrm{T}}>20 \mathrm{GeV}$ with exactly one associated track. The probability of electrons to be misidentified as 3-track $\tau$ jets is negligible. The pair with the highest scalar $E_{\mathrm{T}}$ sum is chosen from all possible $e-\tau$ pairs that are separated by $\Delta R>0.4$. Additionally, the tag and the probe objects are required to have opposite electric charges. Events with $E_{\mathrm{T}}^{\text {miss }}>20 \mathrm{GeV}$ are discarded to reduce the background contamination from $W \rightarrow e v$ decays, and the invariant mass of the $e-\tau$ pair is required to be between 80 and 100 GeV .

The selected probe sample of $\tau$ jet candidates then contains electrons originating from $Z$ bosons with a purity (estimated from simulation) of about $99 \%$. The main backgrounds are multi-jet events, $W \rightarrow e v$, and $Z / \gamma^{*} \rightarrow \tau \tau$, in that order. The multi-jet background is estimated using a two-dimensional sideband subtraction method [39], the electroweak backgrounds using simulation.

Results The misidentification probabilities (as defined in Eq. 3) are extracted for the $\tau$ candidates which pass the $\tau$ selection (including overlap removal with electron candidates) and the electron veto criteria as used in the $H^{+}$selection. In the denominator, the probe objects are not required to pass the $\tau$ jet identification, whereas the numerator contains the number of events with the probe objects both passing the identification and not being discarded by the electron veto. The results for the scale factor and misidentification probability are shown in Table 3 for the different calorimeter regions. Only the scale factors are used in the following. No significant dependence of the scale factor on the $p_{\mathrm{T}}$ of the $\tau$ lepton candidate is observed.

Application of the method to estimate the $e \rightarrow \tau$ misidentification background The misidentification probability from this study is applied by scaling simulated events in which the selected reconstructed $\tau$ jet originates from a true electron. The scale factor used is given by the ratio of the misidentification probability in data to that in Monte Carlo.

Table 3: Scale factors and measured $e \rightarrow \tau$ misidentification probabilities for $\tau$ candidates with $E_{\mathrm{T}}>20$ GeV in the barrel $(0<|\eta|<1.37)$, transition $(1.37<|\eta|<1.52)$ and end-cap $(1.52<|\eta|<2.5)$ regions passing the $\tau$ identification and a tight electron veto, for a $\tau$ identification efficiency of about $30 \%$. The scale factors are given with statistical and systematic uncertainties combined.

| Region | Scale factor | Misidentification probability (data) |
| :--- | ---: | ---: |
| $0<\|\eta\|<1.37$ | $1.1 \pm 0.3$ | $0.0028 \pm 0.0006$ |
| $1.37<\|\eta\|<1.52$ | $1.0 \pm 1.0$ | $0.0005 \pm 0.0004$ |
| $1.52<\|\eta\|<2.5$ | $1.6 \pm 0.5$ | $0.009 \pm 0.003$ |

Systematic uncertainties Five main sources of systematic uncertainties on the electron- $\tau$ jet misidentification probability are studied. The systematic uncertainty due to the subtraction of multi-jet and electroweak backgrounds is at the level of only $1 \%$, but can reach up to $25 \%$ in the transition region. Ideally, the measurement should be independent of the tag selection. To test any potential correlation, this selection has been varied (using medium electron identification criteria instead of tight ones in order to study the bias of only selecting very well-reconstructed tag electrons), leading to an estimate of a systematic uncertainty of $10 \%$. Other systematic uncertainties are negligible in comparison. The choice of the mass window size around $m_{Z}$ applied to the tag-and-probe objects which could result in a bias by only studying objects with well-reconstructed momentum and the uncertainty of the electron energy scale (via the cut on the tag electron energy) only give a small contribution. The total uncertainties on the scale factors (combining the statistical and systematic uncertainties of the measurement) are $24 \%$ in the barrel, $29 \%$ in the end-caps, and $100 \%$ in the transition region. Except for the end-cap, they are dominated by the statistical uncertainties.

In total, the expected contribution of events with electrons misidentified as $\tau$ jets in the signal region is about 2 events which is about $5 \%$ of the expected background. Thus reducing the relatively large uncertainties would only lead to a minor improvement of the $H^{+}$sensitivity.

### 5.1.2 Jet-to- $\tau$ misidentification probability from photon+jets

To study the probability for jets to be misidentified as hadronically decaying $\tau$ leptons, a $\gamma$-jet control sample is used. Like jets from the hard process in the dominant $H^{+}$background $t \bar{t}$, jets in this control sample originate predominantly from quarks as opposed to gluons. A measurement of the probability for a jet to be misidentified as a hadronically decaying $\tau$ lepton is performed using $1.03 \mathrm{fb}^{-1}$ of data and is used to predict the yield of jet-to- $\tau$ misidentification events from the most important SM backgrounds with intrinsic $E_{\mathrm{T}}^{\text {miss }}$. The main difference between $t \bar{t}$ and $\gamma$-jet events is the different fraction of $b$ jets which is smaller in $\gamma$-jet events. However, the probability for a $b$ jet to be misidentified as a $\tau$ jet is smaller than the corresponding probability for a light-quark jet: The average track multiplicity of $b$ jets is higher, and variables which measure the mass of the $\tau$ candidate allow a good discrimination. Hence using the $\gamma$-jet misidentification probability leads to a higher background estimate and is thus conservative.


Figure 2: Jet $\rightarrow \tau$ misidentification probability measured from $\gamma$-jet events for jets with 1 or 3 associated tracks as a function of $p_{\mathrm{T}}$ and $\eta$. The error bars indicate the size of the statistical uncertainties.

The Method Events are required to pass a single-photon trigger (with an $E_{\mathrm{T}}$ threshold of 15,20 or 40 GeV ). The photon candidate must be isolated (less than 6 GeV of $E_{\mathrm{T}}$ deposited in a $\Delta R=0.2$ cone around the photon), is required to match a trigger object, pass the photon selection [40], and have either zero or two associated tracks to include photon conversions. The photon candidate must have $|\eta|<2.37$, not be located in the transition region, and must have a transverse energy of at least 15 GeV . The selected $\gamma$-jet sample consists of events with one photon candidate and a jet with $p_{\mathrm{T}} \geq 20 \mathrm{GeV}$, separated in $\phi$ by at least 2.84 radians. The difference in transverse energy between the jet and the photon must be less than half of the total transverse energy of the photon. Any additional jets are required to have less than $20 \%$ of the photon transverse energy.

The misidentification probability is measured as a function of both $p_{\mathrm{T}}$ and $\eta$. The denominator of the calculated misidentification probability is the number of events with a $\tau$ candidate (i.e. no $\tau$ ID applied) with $p_{\mathrm{T}}$ greater than 20 GeV and $|\eta|<2.3$, which passes an electron veto. The misidentification probability is evaluated separately for the case of candidates with 1 or 3 associated tracks. Among all jets with $E_{\mathrm{T}}>20 \mathrm{GeV}$ and $|\eta|<2.3$, the fraction of light-quark jets which are considered as such $\tau$ candidates is about $27 \%$. The numerator in the calculated misidentification probability consists of events with objects which pass the full $\tau$ identification. They must not be within $\Delta R=0.2$ of any $e$ or $\mu$. The measured misidentification probabilities are shown in Fig. 2.

Systematic uncertainties The dominant systematic uncertainties on the misidentification probability are (the ranges given on each systematic uncertainty show the variation with the $p_{\mathrm{T}}$ and $\eta$ of the $\tau$ candidate):

- Contamination of the control sample with true $\tau$ jets from $Z \rightarrow \tau \tau$ and $W \rightarrow \tau v$ events, evaluated using simulation: $(1-3) \%$.
- Contamination of the control sample with multi-jet events which have a larger gluon-initiated jet fraction than $\gamma$-jet events. The associated systematic uncertainty is evaluated by modifying the photon ID requirements, in particular loosening the photon isolation which increases the impurity from multi-jet events in the control sample: $(5-9) \%$.
- Contamination of the control sample by three-jet events. The associated systematic uncertainty is evaluated by varying the selection cuts (vetoing events with additional jets with less than 0.1 of the
photon momentum), and by splitting the control sample in a part which fulfills even tighter requirements and one which does not, and then taking the variation of the misidentification probability due to these changes as the uncertainty: $(11-17) \%$.
- The measurement of the misidentification probability on the probe object is assumed to be uncorrelated from the selection of the tag object. To evaluate uncertainties from a violation of this assumption, correlations between the tag and the probe objects are studied by changing the requirements on the tag object (requiring a photon with a looser quality criterion) and studying the impact on the measurement of the misidentification probability on the probe object: $(7-14) \%$.

Additionally, the statistical uncertainty of the measurement of the misidentification probability enters as uncertainty on any application of the misidentification probability. The total systematic uncertainty is about $(15-24) \%$, depending on $p_{\mathrm{T}}$ and $\eta$. The systematic uncertainties on the misidentification probability are propagated into the background prediction for the baseline selection and enter the statistical evaluation as shape uncertainties.

Application to estimate the jet $\rightarrow \tau$ misidentification background To predict the background in $\mathrm{H}^{+}$ searches, the measured jet $\rightarrow \tau$ misidentification probability is applied to simulated $t \bar{t}$, single-top, and $W+$ jets events. These events are required to pass the full event selection except for the $\tau$ identification. For these events, $\tau$ candidates fulfilling the same requirements as in the misidentification probability definition which do not overlap with a true $\tau$ lepton are identified. Out of the remaining $\tau$ candidates, each one is considered to be potentially misidentified as a $\tau$ jet separately. The identified jet that corresponds to the $\tau$ candidate is removed from the event, affecting the number of reconstructed jets, the $E_{\mathrm{T}}^{\text {miss }}$ significance of the event, and the number of $b$-tagged jets. If, after taking this into consideration, the event still passes the selection, then the event is counted as background event with a weight given by the misidentification probability corresponding to the $p_{\mathrm{T}}$ and the $\eta$ of the $\tau$ candidate. The predicted number of events from the $t \bar{t}$ sample, together with a comparison to the MC prediction using truth information, is shown in Table 4. All other jet $\rightarrow \tau$ misidentification backgrounds with intrinsic $E_{\mathrm{T}}^{\text {miss }}$ are at least two orders of magnitude smaller than $t \bar{t}$.

Table 4: Application of the misidentification probability obtained from $\gamma$-jet events. The numbers shown are the expected number of events in collision data after the $H^{+}$selection. The prediction based on the misidentification probability measurement (statistical and systematic uncertainties), as well as the MC prediction (statistical uncertainties), are given.

| Sample | Data-driven prediction [number of events] | MC prediction [number of events] |
| :--- | :--- | :--- |
| $t \bar{t}$ | $2.8 \pm 1.0($ stat $) \pm 0.5($ syst $)$ | $3.8 \pm 0.6($ stat $)$ |

### 5.2 Multi-jet background estimate

As the uncertainties on the multi-jet expectation are large, it is necessary to avoid using any multi-jet simulation to estimate this background. Thus an approach different from estimating the jet $\rightarrow \tau$ misidentification contribution in events with intrinsic $E_{\mathrm{T}}^{\text {miss }}$, as described in the previous section, is chosen.

The Method The multi-jet background is estimated by fitting its $E_{\mathrm{T}}^{\text {miss }}$ shape (and the $E_{\mathrm{T}}^{\text {miss }}$ shape of other backgrounds) to data. In order to study this shape in a data-driven way, a control region is defined
where the $\tau$ identification and $b$-tagging requirements are inverted. The $\tau$ candidates must pass a loose $\tau$ identification but fail the tight $\tau$ identification used in the baseline selection. In addition, the event is required not to contain any $b$-tagged jets and therefore also the requirement on the $q q b$ mass (selection cut 7) is removed.

Assuming that the shapes of the $E_{\mathrm{T}}^{\text {miss }}$ and $m_{\mathrm{T}}$ distributions are the same in the control sample and signal regions (see Fig. 3 for a comparison early in the selection cut flow), the shape of the $E_{\mathrm{T}}^{\text {miss }}$ distribution is used to model the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution for the multi-jet background (after subtracting the background from other processes). The $E_{\mathrm{T}}^{\text {miss }}$ distribution measured in data (for the baseline selection) is then fitted using two shapes: this multi-jet model, and the sum of other processes (dominated by $t \bar{t}, W+\mathrm{jets}$ ) for which the shape and the relative normalisation are taken from MC simulation. The free parameters in the fit are the overall normalisation (to the one in data) and the multi-jet fraction.


Figure 3: Distribution of $E_{\mathrm{T}}^{\text {miss }}$, after subtracting the expectation from $t \bar{t}, W+\mathrm{jets}$, and single-top simulation; compared are the distributions after requirement 3 of the baseline selection as detailed in Section 4, with the exception that in the control region, the $\tau$ selection and the $b$-tagging requirements have been inverted. The shaded area indicates the size of the statistical uncertainties.

Systematic uncertainties The dominant systematic uncertainties are:

- The uncertainty on the assumption that the $E_{\mathrm{T}}^{\mathrm{miss}}$ shape is identical in the signal and control regions. This is studied by varying the number of entries in each bin separately within the maximum differences observed early in the selection cut flow (a factor of 0.5 and 2.0) and redoing the fit. Then, the largest downwards and upwards fluctuations are used as systematic uncertainty. This leads to an uncertainty on the multi-jet fraction of $-13 \% /+25 \%$.
- The uncertainty on the $t \bar{t}$ and $W+$ jets shapes and relative normalisation from Monte Carlo is dominated by uncertainties on the $t \bar{t}$ cross section. The scaling of the $t \bar{t}$ Monte Carlo is varied according to these uncertainties, leading to an uncertainty on the multi-jet fraction of $2.4 \%$.
- The uncertainty from backgrounds other than $t \bar{t}$ and $W+$ jets in the control region is found to be negligible.

The uncertainty on the multi-jet fraction is dominated by the statistical uncertainty of the data set on which the fit is performed.

Result of the data-driven estimate of the multi-jet background The multi-jet fraction is estimated to be $(23 \pm 10) \%$ using the fit to the $E_{\mathrm{T}}^{\text {miss }}$ distribution shown in Fig. 4. The $m_{\mathrm{T}}$ distribution for the same
events is shown in Fig. 5. Except for the multi-jet background, all other processes have $W$ bosons in the final state and their distributions drop off around the $W$ boson mass, as expected. Such behavior is neither expected nor observed for the multi-jet background as resulting shapes are mainly caused by detector effects. To probe the region with large $m_{\mathrm{T}}$, in which a potential $H^{+}$signal resides, it is thus important to suppress the multi-jet background as much as possible.


Figure 4: Multi-jet estimate: A fit to the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution in data after all selection cuts using two shapes (one for the multi-jet model, and one for all other background processes, dominated by $t \bar{t}$ and $W+$ jets) is shown. The multi-jet fraction estimated after all selection cuts is $(23 \pm 10) \%$.


Figure 5: Contribution of multi-jet events to the $m_{\mathrm{T}}$ distribution after all cuts of the $H^{+}$selection. The multi-jet fraction is estimated using the fit to the $E_{\mathrm{T}}^{\mathrm{miss}}$ distribution shown in Fig. 4.

### 5.3 Embedding method

Complementary to the methods based on misidentification probability, an embedding method is used for estimating the background from true $\tau$ jets, described below. The method consists of collecting a control sample of $t \bar{t}$, single-top, and $W+$ jets events with a muon in data, and replacing the detector signature of this muon with that of a simulated $\tau$ lepton. The reconstruction is re-applied to the new hybrid
events which are then used to estimate the background to the $H^{+}$selection. The advantage is that the whole event (except for the $\tau$ jet) is taken directly from data, including the underlying event and pile-up, missing energy, $b$-quark jets and light-quark jets. The method has been validated in $\tau+$ jets events using early ATLAS data [41].

### 5.3.1 The Method

Control sample selection To select the $t \bar{t}$-like $\mu+$ jets control sample from data, the following event selection is used:

- Event triggered by a single muon trigger ( $p_{\mathrm{T}}$ threshold of 18 GeV ),
- data quality cuts as described in Section 3,
- exactly one isolated muon with $p_{\mathrm{T}}>25 \mathrm{GeV}$,
- no isolated electron with $p_{\mathrm{T}}>20 \mathrm{GeV}$,
- at least four jets with $p_{\mathrm{T}}>20 \mathrm{GeV}$ in $|\eta|<2.5$,
- at least one of the jets is $b$-tagged (nominal efficiency of $65 \%$ ),
- missing transverse energy $E_{\mathrm{T}}^{\text {miss }}>30 \mathrm{GeV}$,
- scalar sum of energy of reconstructed objects $\sum E_{\mathrm{T}}>200 \mathrm{GeV}$.

This selection is looser than the selection defined in Section 4 in order not to bias the control sample. This also applies to the $\tau$ jet which carries the momentum of the selected muon minus the momentum of the neutrino in the $\tau$ lepton decay and its $p_{\mathrm{T}}$ is required to be larger than 35 GeV in the $H^{+}$selection. The impurity from the background with muons produced in $\tau$ decays, and non-isolated muons (dominantly $b \bar{b}$ and $c \bar{c}$ events) is at the level of $10 \%$ and biases the shape of embedded events. However, the bias is greatly reduced as these events are much less likely to pass the $H^{+}$selection.

Embedding step After events have been selected, the actual embedding step takes place. The muon in the event is selected and its vertex position and momentum are extracted. The momentum is then rescaled to account for the higher $\tau$ lepton mass and fed into TAUOLA to produce the $\tau$ lepton decay products and generate final state radiation. The result is propagated through ATLAS detector simulation, followed by reconstruction. In the next step, tracks, calorimeter deposits and segments in the muon spectrometer in the vicinity of the muon are replaced with those of the simulated $\tau$ lepton decay products.

Comparison of embedding method versus simulation To test the method, the embedded data events are compared to simulated $t \bar{t}$ events (hereafter referred to as 'reference') in which the $\tau$ lepton comes directly from simulation of the whole event, and is not added via the embedding method. To make sure the set of events is comparable, both for the embedded and the reference events, a reconstructed $\tau$ candidate which is matched to a true $\tau$ lepton is required (this can be performed using embedded events, as the $\tau$ part of the event is taken from simulation).

A comparison of distributions of variables relevant to this analysis is shown in Fig. 6. A good agreement is observed within the statistical uncertainties.


Figure 6: Validation plots for the embedding method used to estimate the background with true $\tau$ jets. Embedded data is compared to $t \bar{\tau}$ simulation after applying the $H^{+}$selection. The $\tau$ likelihood (TauLLH), the $\tau$ transverse momentum, the missing transverse energy, and the top quark transverse momentum on the $t \rightarrow b q q$ side are shown. The plots are normalized to unit area. The shaded area indicates the size of the statistical uncertainties on the MC simulation.

### 5.3.2 Application to estimate the true- $\tau$ background

The contribution of backgrounds with true $\tau$ jets to the final $m_{\mathrm{T}}$ distribution is estimated from this distribution for embedded events. The normalisation is taken from collision data events in the region $0-40 \mathrm{GeV}$ of this distribution, where any signal contamination would be low for the expected range of sensitivity $\left(\operatorname{BR}\left(t \rightarrow b H^{+} \approx 5 \%\right)\right)$. Such a contamination is dealt with in the limit-setting process by subtracting the expected signal from the observed data before normalizing the shape to the region $m_{\mathrm{T}}<40 \mathrm{GeV}$. This is done when evaluating the signal+background hypothesis and takes the tested $\mathrm{BR}\left(t \rightarrow b H^{+}\right)$into account. Effectively, this brings the signal+background expectation closer to the background-only expectation.

The following procedure is applied:

1. Apply the $\tau+$ jets event selection to embedded events to obtain the $m_{\mathrm{T}}$ shape.
2. From collision data, count the number of events in the $m_{\mathrm{T}}$ distribution between $0-40 \mathrm{GeV}$ after subtracting the background from objects misidentified as $\tau$ jets.
3. Using this number, normalize the $m_{\mathrm{T}}$ distribution from embedded events using the ratio of events in collision data and embedded data.

For technical reasons, the trigger simulation cannot be re-run for embedded events. As the number of events entering the embedding control sample and passing the whole event selection is still relatively small, the event selection applied to the embedded events is modified by requiring a $\tau$ identified using loose criteria. This can be done because the $m_{\mathrm{T}}$ distribution is normalized to data and, as Fig. 7 (left) shows, the looser cuts do not bias the shape significantly.

The result is shown in Fig. 7 (right). As can be seen, the uncertainty of the background estimate is currently limited by the statistical uncertainty due to the limited number of events in the $t \bar{t}$ control sample. In the range $40<m_{\mathrm{T}}<300 \mathrm{GeV}$, there are $21 \pm 5$ background events with true $\tau$ jets expected where the uncertainty is due to the limited number of events in the control sample, and of the data in the region to which the shape is normalized to. In data, 26 events are observed after subtracting the background predicted by the misidentification probability methods and the multi-jet estimate. Within statistical uncertainties, the background prediction and data agree well.

### 5.3.3 Systematic uncertainties

The following systematic uncertainties are associated with the background prediction:

- To study the effect of additional multi-jet background on the embedding and the control sample selection itself, the $\mu$ isolation requirement is varied. To study a potential bias introduced by the embedding method parameters chosen, alternative values are used for the inner and outer cone size in which calorimeter cell depositions are replaced or added. To account for the fact that a small amount of pile-up-related activity can be present in the calorimeter cells removed in a cone around the muon, the effect of only removing half of this energy before adding the $\tau$ jet is studied. This results in a systematic uncertainty of $7 \%$ on the background normalisation.
- The systematic uncertainty due to the difference in the $m_{\mathrm{T}}$ shape as a consequence of loosening the selection with respect to the $H^{+}$selection, as shown in Fig. 7, results in a $8 \%$ uncertainty on the background normalisation, and a shift of about 2 GeV in the $m_{\mathrm{T}}$ distribution.
- The impact of the incomplete treatment of the $\tau$ polarisation in embedded events results in an uncertainty on the $m_{\mathrm{T}}$ shape which is estimated by comparing bin by bin the difference in the number of events for simulated $t \bar{t}$ events with and without correct treatment of the $\tau$ polarisation.


Figure 7: Left: Comparison of the $m_{\mathrm{T}}$ shape for simulation and for embedded events (with loose $\tau$ identification) used to estimate the background with true $\tau$ jets. The distribution from simulation is shown both after the $H^{+}$baseline selection and after the same selection but without trigger requirement and loose $\tau$ identification. All distributions are normalized to unit area. Right: Comparison of the $m_{\mathrm{T}}$ shape for embedded events versus collision data. The prediction using the embedding method is stacked on top of the expected backgrounds with objects misidentified as $\tau$ jets: MC expectation for $t \bar{t}$ and electroweak processes, and the data-driven estimate for multi-jet events. The comparison is done after the $H^{+}$event selection and after normalizing the $m_{\mathrm{T}}$ distribution of embedded events to the data distribution in the range $0-40 \mathrm{GeV}$. The gray area indicates the size of the statistical and systematic uncertainties of the embedding method estimate.

This results in an uncertainty on the normalisation of $15 \%$, and the $m_{\mathrm{T}}$ distribution is shifted by about 7 GeV which corresponds to $14 \%$ of the average $m_{\mathrm{T}}$.

- The impact on the $m_{\mathrm{T}}$ distribution due to the uncertainty on the $\tau$ energy scale (Table 2 ) is evaluated, leading to a normalisation uncertainty of $+4 /-2 \%$, and a shift in the $m_{\mathrm{T}}$ distribution by $\pm 1 \mathrm{GeV}$.

The statistical uncertainty of the estimate is $8 \%$ due to the limited size of the control sample, and additionally $20 \%$ due to the normalisation to data (allowing data to fluctuate within one standard deviation for $m_{\mathrm{T}}<40 \mathrm{GeV}$ ). The numbers above are only indicative, for the limit calculation the full shape uncertainty is used.

## 6 Results

The results of the data-driven methods in estimating the contributions of the various categories of backgrounds after the baseline selection are summarized in Table 5, and the $m_{\mathrm{T}}$ distribution of the remaining events is shown in Fig. 8. The total systematic uncertainty on the background prediction is about $30 \%$ but can reach up to $70 \%$ for $m_{\mathrm{T}}>100 \mathrm{GeV}$. For the signal, the total systematic uncertainty on the yield is about $40 \%$ with a small dependence on $m_{H^{+}}$. The number of events with true $\tau$ jets has been estimated with the embedding method, the jet $\rightarrow \tau$ misidentification events with intrinsic $E_{\mathrm{T}}^{\text {miss }}$ with $\gamma+\mathrm{jets}$ control samples, the $e \rightarrow \tau$ misidentification events with $Z / \gamma^{*} \rightarrow e e$ control samples, and the multi-jet contribution by taking its shape from a sideband region and fitting it to the data. The number of events with $m_{\mathrm{T}}>40 \mathrm{GeV}$ is given which allows for a better comparison of data and expectation as the estimate from the embedding method is normalized to data in the range $m_{\mathrm{T}}<40 \mathrm{GeV}$. A good agreement between the estimated and the observed number of events is seen.

Table 5: Expected number of events from data-driven estimates with $m_{\mathrm{T}}>40 \mathrm{GeV}$, and as observed in data. Only statistical uncertainties are given.

|  | Events with/from |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | true $\tau$ jets | jet $\rightarrow \tau$ mis-id | $e \rightarrow \tau$ mis-id | multi-jet | expected (sum) | data |
| $m_{\mathrm{T}}>40 \mathrm{GeV}$ | $21 \pm 5$ | $2.4 \pm 0.7$ | $1.9 \pm 0.2$ | $12 \pm 5$ | $37 \pm 7$ | 43 |

Using data-driven background estimates, no statistically significant excess of events is observed in $1.03 \mathrm{fb}^{-1}$ of collision data. Exclusion limits are set on the branching ratio $t \rightarrow b H^{+}$, and in the $m_{H^{+}}-\tan \beta$ plane, by rejecting the signal hypothesis at the $95 \%$ confidence level applying the $\mathrm{CL}_{s}$ procedure [42, 43]. A profile likelihood ratio [44] is used with the $m_{\mathrm{T}}$ distribution as the discriminating variable. The statistical analysis is based on a binned likelihood function for the $m_{\mathrm{T}}$ distribution. Systematic uncertainties in shape and normalisation are incorporated via nuisance parameters and the one-sided profile likelihood ratio, $\tilde{q}_{\mu}$, is used as a test statistic. The final limits are based on the asymptotic distribution of the test statistic [44].

The resulting exclusion limit is shown in Fig. 9 in terms of $\operatorname{BR}\left(t \rightarrow H^{+} b\right) \times \operatorname{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$. Figure 10 shows the upper limit in the context of the $m_{h}^{\max }$ scenario of the MSSM [45] in the $m_{H^{+-}} \tan \beta$ plane. No exclusion limit is shown for charged Higgs boson masses close to 160 GeV as no reliable calculations for $\mathrm{BR}\left(t \rightarrow H^{+} b\right)$ exist for $\tan \beta$ values in the range of interest. The following relative uncertainties on $\mathrm{BR}\left(t \rightarrow b H^{+}\right)$are considered [46]: 5\% for one-loop electro-weak corrections missing in the calculations, $2 \%$ for missing two-loop QCD corrections, and about $1 \%$ (depending on $\tan \beta$ ) $\Delta_{b^{-}}$ induced uncertainties (where $\Delta_{b}$ is a correction factor to the running bottom quark mass [47]). These


Figure 8: The $m_{\mathrm{T}}$ distribution after event selection. The observation in collision data, and the estimates from data-driven methods are compared. The distribution of the $H^{+}$signal is given for a reference point in parameter space corresponding to $\mathrm{BR}\left(t \rightarrow b H^{+}\right)=10 \%$, thus the SM-like $t \bar{t}$ background is reduced correspondingly.
uncertainties are added linearly. This result constitutes a significant improvement compared to existing limits provided by the Tevatron experiments [6] over the whole investigated mass range, but in particular for charged Higgs boson masses close to the top quark mass.

## 7 Conclusions

Charged Higgs bosons are searched for in the decay mode $t \rightarrow b H^{+}, H^{+} \rightarrow \tau v$, with hadronically decaying $\tau$ leptons, using $t \bar{t}$ events reconstructed in a total of $1.03 \mathrm{fb}^{-1}$ of $\sqrt{s}=7 \mathrm{TeV} p p$ collision data recorded with the ATLAS experiment. Data-driven methods, employed to estimate the number of background events characterized by the presence of a $\tau$ jet, $E_{\mathrm{T}}^{\text {miss }}, b$ jets, and a hadronically decaying $W$ boson, predict $37 \pm 7$ (stat) events with $m_{\mathrm{T}}>40 \mathrm{GeV}$. A total of 43 such events are observed which is consistent with the prediction. The $\mathrm{CL}_{s}$ procedure is used to derive $95 \%$ CL exclusion limits. Values of the product of branching ratios, $\mathrm{BR}\left(t \rightarrow b H^{+}\right) \times \mathrm{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$, larger than $0.03-0.10$ have been excluded in the $H^{+}$mass range $90-160 \mathrm{GeV}$, significantly extending limits from other experiments. Interpreted in the context of the $m_{h}^{\max }$ scenario of the MSSM, values of $\tan \beta$ above $22-30$ (depending on $m_{H^{+}}$) can be excluded in the mass range $90 \mathrm{GeV}<m_{H^{ \pm}}<140 \mathrm{GeV}$.

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Figure 9: Expected and observed $95 \%$ CL exclusion limits for charged Higgs boson production from top quark decays as a function of $m_{H^{+}}$in terms of $\mathrm{BR}\left(t \rightarrow H^{+} b\right) \times \mathrm{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$. For comparison, the best limit provided by the Tevatron experiments is shown [6].


Figure 10: Limit for charged Higgs boson production from top quark decays in the $m_{H^{+-}} \tan \beta$ plane. Results are shown for the MSSM scenario $m_{h}^{\max }$.
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## A Limit figure with PCL



Figure 11: Expected and observed $95 \%$ CL exclusion limits for charged Higgs boson production from top quark decays as a function of $m_{H^{+}}$in terms of $\mathrm{BR}\left(t \rightarrow H^{+} b\right) \times \mathrm{BR}\left(H^{+} \rightarrow \tau^{+} v\right)$ using the $\mathrm{CL}_{s}$ procedure. Power-Constrained limits (PCL) [48] with a $50 \%$ power constraint are shown as well. For comparison, the best limit provided by the Tevatron experiments is shown [6].

## 3. D0 Experiment at Tevatron

SMU joined the D0 Experiment in 2004, following a long D0 involvement by Kehoe since 1992. The primary thrust of the SMU project has been to study top quark physics ultimately to probe electroweak symmetry breaking, particularly in the period before a Higgs boson discovery. Kehoe's early efforts at SMU were to measure the top quark pair cross section, but have primarily focused on measuring the top quark mass. This activity was supported by work on the Level 1 Calorimeter upgrade for Run 2b (2004-2006), work by SMU postdoc Renkel to co-coordinate the Common Samples Group (20102011), and jet energy calibration efforts for the final data sample (2011-2013).

Recent activities by our group have involved postdocs Renkel and Amitabha Das, and Ph.D. students Yuriy Ilchenko and Huanzhao Liu. Our primary effort was top quark mass measurement and jet energy calibration. The effort has been productive, yielding conference and journal papers on top quark mass measurement, and on modelindependent searches for new physics. Ilchenko is now a postdoc at $U$. of Texas, Austin on ATLAS.
a) Jet Energy Scale (Liu, Ilchenko, Das, Kehoe): The JES is critical to the measurement of the top quark mass. The primary calibration is extracted using $\mathrm{E}_{\text {Tmiss }}$ in $\gamma+\mathrm{jet}$ events. SMU has major involvement in several elements of the standard D0 JES. In data, the $\gamma+$ jet signature has substantial instrumental background. To calibrate data to the same level as MC, we must evaluate the purity of the photon sample, correct the scale appropriately and establish a systematic uncertainty. Ilchenko studied the photon purity for data after the 2006 upgrade ('R2b') as it applies to the jet response ( $R_{j}$ ) measurement in the central region. The purity is evaluated with a template fit using an isolation variable from tracks near the photon. He determined a new efficiency for data and improved the statistical error calculation. He measured the purity for all of R2b and resolved a difficulty with poor $\chi^{2}$ in pre-shutdown data ('R2a').

D0 calibrates jets in data and MC independently using similar methods. He studied the ratio of the $R 2 a$ and $R 2 b$ MC jet responses vs. $E^{\prime}=\mathrm{p}_{\mathrm{T}^{* *}} \cosh \left(\eta_{\mathrm{j}}\right)$ in several $\eta$ bins and established agreement within quoted systematics. Liu and Kehoe continued with a study of $\Delta R=0.5$ cone jets and $M C$ simulating the luminosity profile of all $R 2 b$ run ranges. We observed excellent agreement within R 2 b and good agreement relative to R2a, although at low and very high energies a difference was observed that was still within the existing systematic uncertainty band. Liu observed no dependence on the number of primary vertices or on central preshower requirements for the photon. He also studied potential biases from the fitting method to develop a correction for data. He determined the absolute $R_{j}$ in MC for all R 2 b MC run ranges. The response is stable to within 1\% (see Figure 11).

The D0 detector is uniform in LAr calorimetry except for the inter-cryostat region occupied by scintillators (ICD). Liu derived $\eta$-dependence corrections for all run periods in data using $\gamma+$ jet and dijet events to maximize the energy reach out to $|\eta|=3.6$. He also used the $\chi^{2}$ to calculate the systematic uncertainty while avoiding double counting statistical uncertainties. The relative uncertainty is $<1.5 \%$ in most of the detector. This correction, and the purity and MC scale corrections, are now included in the final
corrections for the full data sample. Das performs the final data closure tests of the effectiveness of the overall calibration by computing the ratio of the corrected reconstructed jet energies between data and $\mathrm{MC} \gamma+$ jet events in photon $\mathrm{p}_{\mathrm{T}}$ bins. He sequentially identified and helped resolve several inconsistencies and bugs in the calibration software, and he established the ratio to be around 1 , with $\sim 2 \%$ uncertainty. The final jet energy scale step entails a post-calibration jet smearing and scaling correction. Das implemented this for the full data sample and worked to complete this final part of the jet energy scale analysis. Liu, Ilchenko, Das and Kehoe contributed to the final analysis note describing this work [1], and each wrote portions of the draft NIM paper currently in internal review.

### 3.4 D0 Physics Analysis:

The top quark mass, $m_{t}$, is a fundamental parameter of the SM and it provides sensitivity to the SM Higgs boson mass through radiative corrections. Its value indicates a Yukawa coupling near unity, which may point to new physics. Our effort on D0 has been focused on a precision measurement of the top mass in dilepton events. A model-independent search for new physics was also pursued.
a) Top Quark Mass in Dilepton Events (Renkel, Kehoe, Ilchenko, Liu, Das): Mass analysis in dilepton events is challenged by loss of kinematic information to two neutrinos and by the absence of $\mathrm{W} \rightarrow \mathrm{jj}$ in the final state. Since our result in $1 \mathrm{fb}^{-1}$ [2], we analyzed $4.3 \mathrm{fb}^{-1}$ of $\mathrm{R} 2 \mathrm{~b} e \mu$ events. We integrate over the expected neutrino $\eta$ distribution and compare the solved momenta to the observed $\mathrm{E}_{\text {Tmiss }}$ to obtain a relative weight vs. $m_{t}$. Ilchenko rewrote the weight calculation, and he and Kehoe fitted the $\eta$ distribution and optimized the binning of this distribution to balance CPU time with improvement in the statistical error expected in pseudo-experiments. He and undergraduate Jason South tested fitting the $\eta$ distribution with different functions, and developed a linear parametrization of the width of the $\eta$ distribution with $m_{t}$. We measure $m_{t}$ by fitting 3D templates relating the first two moments of the weight distribution with $m_{t}$. Liu and Kehoe optimized template binning to minimize the expected statistical error. Renkel estimated most systematic uncertainties and improved the treatment of statistical errors to better reflect MC samples. We obtained the world's most precise $m_{t}$ in dilepton events [3]. The results were shown at HCP 2010, and by Renkel at HQL 2010. Kehoe presented top and EWK at the Fermi User's Meeting, 2010.

This measurement was limited particularly by JES uncertainties. Renkel and Kehoe focused on a more accurate JES determination from analysis of $\mathrm{W} \rightarrow \mathrm{jj}$ in $t \bar{t}$ single lepton+jets (' $1+$ jets') events. We had to account for the different event topologies of dilepton and $1+$ jets events that can cause slight differences in JES. Renkel used single particle responses for data and MC to calculate their ratio in dilepton events, and in $1+$ jets events. The ratio of these ratios indicates agreement to within $0.3 \%$ (see Figure 11) and is taken as a systematic uncertainty. The shift is primarily because the b-jet particle multiplicity in the two samples differs by a few percent. Renkel implemented the $1+$ jets scale from $2.6 \mathrm{fb}^{-1}$ into the analysis, plus a time-dependent correction for aging of ICD since that analysis. Also for the first time in dilepton events, he implemented corrections to bring the flavor dependence of the MC JES into agreement with data. After several studies, only the overall calorimeter time-dependence was a significant ( $0.7 \%$ ) source of
uncertainty. Renkel also performed the residual JES uncertainty determinations for kinematic and flavor differences of dilepton b-jets relative to jets from $\mathrm{W} \rightarrow \mathrm{jj}$.



Figure 1: Central $\boldsymbol{R}_{\boldsymbol{j}}$ vs. $\mathrm{E}^{\prime}$ in MC for three different D0 run periods (left). Measured double ratio in the DO dilepton sample vs. $l+$ jets sample (right).

Ilchenko applied the new JES to $e e, e \mu$ and $\mu \mu$ channels. He also performed several studies to improve the statistical sensitivity of the analysis. While they did not reveal a clear improvement, they provided valuable insight motivating current studies by Liu. Ilchenko was primarily responsible for performing the full analysis, from selection, to moments calculation, fitting, testing and most systematics. He and Kehoe also performed a detailed analysis of high $\chi^{2}$ values in calibration plots, which were determined to arise from oversampling and varying Alpgen weights. Accounting for these caused no significant shift to the method's calibration. Our final result of $174.0 \pm 2.4($ stat $) \pm 1.4$ (syst) GeV in $5.3 \mathrm{fb}^{-1}$ [4] is included in the Tevatron $m_{t}$ average [5]. This was the first time the $\mathrm{W} \rightarrow \mathrm{jj}$ resonance has been used to calibrate jets outside the parent $1+$ jets sample. Ilchenko and Liu presented these results at Lake Louise and APS, respectively. Ilchenko is finishing his dissertation. Renkel presented top results at HQL and Aspen. Kehoe gave an invited talk on Top Quark Physics for Tevatron at APS. Das and Kehoe determined correlations between SMU and matrix-element approaches in R2a and R2b. Combining these analyses slightly improves our precision, giving the world's smallest uncertainty ( $1.4 \%$ ) in dilepton events [6]. This was published in fall.

With jet calibration and previous analysis finished, we have worked to analyze the full Run 2 b data sample of $8.7 \mathrm{fb}^{-1}$. Das set up the skimming software to extract this data sample. He worked through several difficulties particularly with the most recent data, and validated the output against previous results. He and Kehoe also worked with Liu in developing ideas to improve or modify the neutrino weighting approach to increase its statistical power. Liu has developed several techniques that improve the numerical integration, and more effectively identify correct jet-lepton assignments and neutrino solutions. He has run the full data sample with the old jet energy scale to verify results against our earlier measurement. Skimming with the new jet energy scale, and tests of the method sensitivity were also completed.
b) Model Independent Search for New Physics (Renkel): Renkel pursued a modelindependent search in over 120 channels in collaboration with Michigan State. He made substantial contributions, including his focus on applying MC corrections for tagging of
b-jets because many final states had b-jets. Space limitations preclude a more detailed discussion. He was integrally involved in EB and referee responses [7]. He presented results at DPF 2011 and SUSY 2011.
c) Other D0 Activities: Renkel was MC representative for the Top and JES groups, and co-convenor of DØ's Common Samples Group (CSG) in 2010-2011. The Top/JES job entailed developing MC requests within the groups, requesting and validating the samples, and developing infrastructure for special requests. As CSG convenor, a major D0 responsibility, Renkel's work included processing the data, maintaining databases, and calculating luminosity profiles for MC samples. Kehoe co-chaired the editorial board reviewing lifetime and CP -violation measurements in the $\mathrm{B}_{\mathrm{s}}$ system through 2011. Highlights were analyses of $\mathrm{B}_{\mathrm{s}} \rightarrow \mathrm{J} / \psi \phi[8]$ and $\mathrm{B}_{\mathrm{s}} \rightarrow \mathrm{J} / \psi \mathrm{f} 0$ [9]. Renkel, Ilchenko, Liu and Kehoe took calorimeter shifts during data-taking.

## Appendix 1: Bibliography

List of recent D0 notes and publications with significant contributions from SMU authors listed.

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3. [MC]: Measurement of the Top Quark Mass in em Final States with Neutrino Weighting in Run II at D0, D0-CONF-6104 (2010).
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5. [MV]: Combination of Top Quark Mass Measurements from the Tevatron Collider, D0+CDF Collabs., Phys. Rev. D 86:092003 (2012).
6. [M]: Measurement of the Top Quark Mass in ppbar Collisions Using Events with 2 Leptons, Abazov, et al., Phys. Rev. D Rapid Comm. 86:051103 (2012).
7. [MI]: Model-independent Search for New Physics in ppbar Collisions at sqrt(s)=1.96 TeV, Abazov, et al., Phys. Rev. D 85:092015 (2012).
8. [B1]: Measurement of CP-violating phase $f^{J / v f}$ using flavor-tagged decay $B_{s^{-}}>J / y f$ in 8 $\mathrm{fb}^{-1}$ of ppbar collisions, Abazov, et al., Phys. Rev. D 85:032006 (2012).
9. [B2]: Measurement of the relative branching ratio of Bs->J/yf0 Bs->J/yf, Abazov, et al., Phys. Rev. D 85:011103 (2012).

# Measurement of the Mass of the Top Quark in $e \mu+$ Jets Final States at DØ with $5.3 \mathrm{fb}^{-1}$ 

The DØ Collaboration<br>URL http://www-d0.fnal.gov<br>(Dated: August 25, 2010)


#### Abstract

We present a measurement of the mass of the top quark $\left(m_{\mathrm{t}}\right)$ in $e \mu+2$ jets final state using data corresponding to $5.3 \mathrm{fb}^{-1}$ collected by the $\mathrm{D} \varnothing$ experiment at the Fermilab Tevatron. The mass is extracted from an analysis of $t \bar{t} \rightarrow b W^{+} \bar{b} W^{-} \rightarrow b \bar{b} \mathrm{e}^{ \pm} \mu^{\mp} \nu_{\mathrm{e}} \nu_{\mu}$ candidate events. We employ a comparison of expected properties of the two unobserved neutrinos with the imbalance in transverse momentum in data, as a function of $m_{\mathrm{t}}$.

We measure $m_{\mathrm{t}}=173.3 \pm 2.4$ (stat.) $\pm 2.1$ (syst.) GeV by combining a Run2b top quark mass measurement with $4.3 \mathrm{fb}^{-1}$ and a Run2a measurement with $1.0 \mathrm{fb}^{-1}$.


## I. INTRODUCTION

In the standard model $(S M)$, the masses of vector bosons are generated from spontaneous breaking of electroweak symmetry, and masses of fermions arise from their Yukawa couplings to the scalar Higgs field [1]. In $S M$, we can use top quark mass, and $W$ boson mass to constraint the Higgs boson mass.

In this analysis, we measure $m_{\mathrm{t}}$ in $e \mu+$ jets decays of $t \bar{t}$ pairs. Each top quark decays to $W b$ with a branching fraction close to $\sim 100 \%$, and each $W$ boson decays into either a lepton and a neutrino, or two quarks. In the present analysis, we consider just those final states with one electron and one muon. They can arise from either $W \rightarrow e(\mu) \nu$, or from $W \rightarrow \tau \nu \rightarrow e(\mu) \nu \nu$ decays.

The value of $m_{\mathrm{t}}$ is measured in $4.3 \mathrm{fb}^{-1}$ of data collected at $\mathrm{D} \varnothing$ in Run 2 b of the Tevatron. The $\mathrm{D} \emptyset$ detector is described in Ref. [2]. The presented analysis is based on the Neutrino Weighting method used for $m_{\mathrm{t}}$ measurement in $1 \mathrm{fb}^{-1}$ of Run 2a data [3]. Assuming various top quark masses, the consistency of the observed event kinematics can be used to obtain weights for each event versus top quark mass using simulated neutrino pseudo-rapidity distributions. Weights are calculated for a range of assumed top quark masses based on the consistency of these momenta with the measured event $E_{T}$. We determine $m_{\mathrm{t}}$ using histograms of probability density of the first two moments of the weight distributions for different assumed $m_{\mathrm{t}}$.

## II. SELECTION OF EVENTS

The event selection used for this measurement is similar to the one used to measure the $t \bar{t}$ cross section in the same final state [4]. Basic requirements include one isolated electron and one isolated muon of opposite charge and transverse momenta of at least 15 GeV , exactly two jets that have transverse momenta of at least 20 GeV , and significant $H_{T}$, defined as the scalar sum of the transverse momenta of the two jets and the leading lepton. The only other requirement is that the events must pass the kinematic reconstruction of Section III. Table I shows the expected event yields for signal and backgrounds, as well as the number of events in data before and after kinematic reconstruction. The uncertainties are statistical only except for an uncertainty on signal yield, where it arises due to theoretical uncertainty on the $t \bar{t}$ cross section. The expected yields differ from those from Ref. [4] due to a different $H_{T}$ cut. For our measurement, the $H_{T}$ cut was slightly increased from $H_{T}>110 \mathrm{GeV}$ to $H_{T}>115 \mathrm{GeV}$ to reduce the expected statistical uncertainty on $m_{\mathrm{t}}$.

The signal and $Z \rightarrow \tau \tau$ background processes are generated with ALPGEN [5], followed by PYTHIA [6] for showering and hadronization, the diboson samples (WW,WZ,ZZ) are generated with PYTHIA. Instrumental effects can cause object misidentification, and mismeasurement of missing transverse energy. Instrumental background is modeled using data.

TABLE I: Expected and observed $e \mu$ event yield for background and signal ( $\sigma_{t \bar{t}}=7.45 \mathrm{pb}$ for $m_{\mathrm{t}}=172.5 \mathrm{GeV}$ ), after applying all selections. The numbers in the first six columns are given before the kinematic reconstruction.

| $t \bar{t} \rightarrow e \mu$ | $Z \rightarrow \tau \tau$ | diboson | instrumental | total | observed | after kinematic reconstruction |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $141.6_{-11.4}^{+11.4}$ | $10.9_{-1.3}^{+1.3}$ | $6.2_{-0.7}^{+0.7}$ | $10.8_{-3.8}^{+4.0}$ | $169.5_{-12.2}^{+12.2}$ | 202 | 197 |

## III. METHOD OF ANALYSIS

The kinematic reconstruction is based on the fact that the final state consists of the following six particles: two charged leptons, two jets from the $b$ quarks, and two neutrinos. After the assignments of the mass to each particle in the final state, a total of 18 independent kinematic quantities needed to fully measure the final state. Twelve of these quantities - the momenta of the charged leptons and jets - are measured directly in the detector. Five additional constraints are added by requiring that
(i) the two components of the observed imbalance in missing transverse momentum $\left(\mathbb{E}_{T}\right)$ equal the sum of the respective components of the two neutrinos;
(ii) the invariant mass of each pair of lepton and neutrino equals the $W$ boson mass; and
(iii) the mass of the top quark equals the mass of the antitop quark.

This leads to a total of seventeen constraints, which is one constraint short of providing a solution for the system.
A solution can be found by assuming a value of $m_{\mathrm{t}}$. We use the measured $E_{T}$ in each event to assign a weight to each solution. The weight is based on the agreement of the calculated transverse momentum of the neutrinos and the observed $E_{T}$ :

$$
\begin{equation*}
\omega=\frac{1}{N_{\text {iter }}} \sum_{i=1}^{N_{\text {iter }}} \exp \left(\frac{-\left(E_{x, i}^{\text {calc }}-\mathscr{E}_{x}^{\mathrm{obs}}\right)^{2}}{2 \sigma_{\mathbb{E}_{x}}^{2}}\right) \exp \left(\frac{-\left(E_{y, i}^{\mathrm{calc}}-Z_{y}^{\mathrm{obs}}\right)^{2}}{2 \sigma_{E_{y}}^{2}}\right) \tag{1}
\end{equation*}
$$

The calculated transverse momentum is found by ignoring the measured $E_{T}$, and, instead, assuming a pseudorapidity for each unobserved neutrino. From this input, the 3-momentum of each neutrino can be determined. This process is called a kinematic reconstruction. $N_{\text {iter }}$ indicates a sum over all assignments of jets to leptons and solutions for the kinematic reconstruction. An assigment of a jet to a lepton is an assumption that both of them are final decay products of the same top quark. There are two such assumptions per event. The resolutions for the two components of $E_{T}, \sigma_{E_{x, y}}$, are parameters of the method, and taken to be $6 \mathrm{GeV}[3]$. The top quark mass dependence on this parameter is very mild and does not create any systematic ncertainty. Integrating $\omega$ over the the distribution in $\eta$, $\rho(\eta)$, we obtain an overall weight $W\left(m_{\mathrm{t}}\right)$ as a function of assumed $m_{t}$ :

$$
\begin{equation*}
W\left(m_{\mathrm{t}}\right)=\int \omega\left(\eta_{1}, \eta_{2}\right) \rho\left(\eta_{1}\right) \rho\left(\eta_{2}\right) d \eta_{1} d \eta_{2} \tag{2}
\end{equation*}
$$

The distributions in neutrino pseudorapidity are all modeled as Gaussians, with root-mean-square (rms) of 1.0.
To kinematically reconstruct an event, we have to solve a system of two quadratic equations. If none of the solutions have real values, the event is said to fail kinematic reconstruction. The breakdown in efficiencies for kinematic reconstruction for different event sources is given in Table II. The efficiencies are defined as the ratio of expected event yield before the reconstruction and the yield after the reconstruction.

TABLE II: Efficiencies for kinematic reconstruction of events, with $H_{T}>115 \mathrm{GeV}$ cut.

| sample | $t \bar{t}(172.5 \mathrm{GeV})$ | $\mathrm{Z} \rightarrow \tau \tau$ | diboson | data |
| :---: | :---: | :---: | :---: | :---: |
| efficiency, $\%$ | $98.7 \pm 0.05$ | $96.6 \pm 2.3$ | $92.3 \pm 2.4$ | $97.5 \pm 1.1$ |

Weights calculated for different $m_{\mathrm{t}}$ yield a weight distribution for each event, which depends significantly on the number of sampling points used for each neutrino pseudorapidity distribution. In previous versions of this analysis, we used 10 sampling points. We have tested the analysis using 10 to 200 sampling points of neutrino $\eta$, and find that 29 such points ensure the optimal performance of the method. This sampling results in the desired gain in kinematic reconstruction efficiency and statistical uncertainty on $m_{\mathrm{t}}$ while balancing against CPU requirements. The overall weight $W\left(m_{\mathrm{t}}\right)$ is calculated in 1 GeV increments for $80<m_{\mathrm{t}}<330 \mathrm{GeV}$ by summing over all the weights for each chosen neutrino $\eta$.

## IV. PROBABILITY DENSITY HISTOGRAMS

For each event, $W\left(m_{\mathrm{t}}\right)$ is obtained as a function of the assumed $m_{\mathrm{t}}$. Two parameters are chosen to characterize this distribution for every event [3], namely the mean $\left(\mu_{w}\right)$ and root-mean-square ( $\sigma_{w}$ ) of the distribution. The normalized three-dimensional distribution of $\mu_{w}, \sigma_{w}$, and input $m_{\mathrm{t}}$ yields a signal probability histogram, $h_{s}\left(\mu_{w}, \sigma_{w}, m_{\mathrm{t}}\right)$. The background probability density histogram, $h_{b}\left(\mu_{w}, \sigma_{w}\right)$ which is not a function of $m_{\mathrm{t}}$, is obtained as the two-dimensional distribution of $\mu_{w}$ and $\sigma_{w}$ of simulated background events. Weights are assigned to events of different background sources that correspond to the their relative contributions. Probability density histograms scaled to expected event yields for background $h_{b}\left(\mu_{w}, \sigma_{w}\right)$ and signal $h_{s}\left(\mu_{w}, \sigma_{w}, 175 \mathrm{GeV}\right)$, and dependence of $\mu_{w}$ on $m_{t}$ for $25<\sigma_{w}<35$ are shown in Fig. 1.

## V. MAXIMUM LIKELIHOOD

After having modeled the signal probability histogram, $h_{s}\left(\mu_{w}, \sigma_{w} \mid m_{\mathrm{t}}\right)$, and background probability density histogram, $h_{b}\left(\mu_{w}, \sigma_{w}\right)$, the top quark mass is extracted by maximizing the likelihood:

$$
\begin{equation*}
\mathcal{L}\left(\mu_{\omega\{1 . . \mathrm{N}\}}, \sigma_{\omega\{1 . . \mathrm{N}\}}, N\left|\bar{n}_{b}, \bar{n}_{s}\right| m_{\mathrm{t}}\right)=\prod_{i=1}^{N} \frac{\bar{n}_{s} h_{s}\left(\mu_{\omega i}, \sigma_{\omega i} \mid m_{\mathrm{t}}\right)+\bar{n}_{b} h_{b}\left(\mu_{\omega_{i}}, \sigma_{\omega i}\right)}{\bar{n}_{s}+\bar{n}_{b}} \tag{3}
\end{equation*}
$$



FIG. 1: The calculated probability density histogram scaled to expected event yields for (a) background, (b) signal with $m_{\mathrm{t}}=175 \mathrm{GeV}$ as a function of $\mu_{w}$ and $\sigma_{w}$, and (c) dependence of $\mu_{w}$ on $m_{t}$ for signal.

Here $\bar{n}_{s}$ and $\bar{n}_{b}$ are the expected event yields for signal and background respectively, and $N$ is the total number of selected events. The parameters of the likelihood are broken into three groups: measured, expected, and fitted parameters. Uncertainties on the likelihood appear due to the finite statistics in our signal Monte Carlo samples. The distribution of $-\log \mathcal{L}$ vs. $\mathrm{m}_{\mathrm{t}}$ is fit by a parabola within an interval of $\pm 15 \mathrm{GeV}$ around the likelihood point with the lowest value. Signal sample corresponding to the top quark mass of 155 GeV was not used in the fits and ensemble tests for technical reasons. The value of $\mathrm{m}_{\mathrm{t}}$ at the minimum of the parabola defines our top quark mass estimate, $\hat{\mathrm{m}}_{\mathrm{t}}$. Half the width of the parabola where $-\log \mathcal{L}$ rises to 0.5 units more than its minimum value provides the statistical uncertainty, $\hat{\sigma}_{\mathrm{m}_{\mathrm{t}}}$.

The performance of the mass extraction technique is evaluated using ensemble testing techniques: the top quark mass $m_{\mathrm{t}}$ is extracted in ensembles of pseudoexperiments of 197 events. The events are chosen randomly from the signal and background Monte Carlo samples so that the average number of background events per source matches the expected yield. The actual number of events in a given pseudoexperiment is obtained according to a Poisson distribution. The mean of the Poisson distribution is taken from a Gaussian distribution centered at the expected event yield and with uncertainty equal to the total statistical uncertainty.

We employ two approaches for the ensemble tests. In the first approach, which is used for the measurement, we use the information about signal cross section from theory in Table I for all mass points. We fluctuate signal in the same way as the background processes and we select only those pseudoexperiments for which the total number of events exactly equals those observed in data. We employ 1000 pseudoexperiments in an ensemble, and we correct for the correlations among pseudoexperiments since the events are used in the pseudoexperiments more than once. However, the expected signal cross section may not accurately reflect the actual number of $t \bar{t}$ events in the selected sample. Consequently, the number of $t \bar{t}$ used for the ensemble tests can be incorrect. Also, this number depends on the assumed $m_{t}$. This might lead to a bias in the calibration of measured $m_{t}$. Therefore, we use a second approach [3] as a cross-check. We give up the information on the expected cross section, and the signal event yield in a pseudoexperiment is taken as the number of data events minus the total background event yield. Both approaches give consistent results.

Figure 2 shows a good agreement between the output and input top quark mass for the first approach and demonstrates the validity of the statistical error estimation, with widths of pull distributions near their expected value of 1.0. The linear fits in Fig. 2 are used to calibrate the results from data, mapping the output minimum to an input


FIG. 2: (a) shows the fitted top quark mass as a function of the generated MC input top quark mass with central value of the signal cross section taken from theory and with a correction for resampling MC events, and (b) pull width distributions with the same treatment.
top quark mass. The results of the fits are summarized in Table III. The neutrino pseudorapidity distribution is mass dependent, and our analysis assumes a mass-independent Gaussian of width 1.0. We tested the sensitivity of our analysis to this choice by repeating the analysis with a mass-dependent width fit in MC top samples with generator masses of 130 GeV to 210 GeV . The estimated expected statistical uncertainty changed by only 0.03 GeV . We also checked the stability of the result for variations in the range used in the fit, and the small dependence of the minimum on the width of the window for the fit is included in the calibration uncertainty on the final result.

|  | slope | offset $(\mathrm{GeV})$ | $\langle$ pull width $\rangle$ |
| :---: | :---: | :---: | :---: |
| signal cross section from theory | $0.99 \pm 0.006$ | $0.45 \pm 0.09$ | $1.0 \pm 0.007$ |

TABLE III: Slope and offset of the calibration curve in Fig. 2, and the pull width.

## VI. RESULTS

The top quark mass is estimated by maximizing the likelihood for the selected data. The top quark mass estimate and uncertainties are corrected to account for the calibration from ensemble tests (slope and offset, and pull widths) by using the calibration curves of Fig. 2. The measured top quark mass after calibration yields $m_{\mathrm{t}}=172.73 \pm$ 2.81 (stat.) GeV. The cross-check measurement is within 0.1 GeV of this result.

The negative log likelihood as a function of top quark mass before the calibration, together with the parabolic fit, are shown in Fig. 3. The distribution of expected statistical uncertainties is shown in Fig. 4, overlaid with the value observed in data.

## VII. SYSTEMATIC UNCERTAINTIES

A summary of the systematic uncertainties is given below.
(i) Jet energy scale: We evaluate this systematic uncertainty by shifting the jet energy scale by $+1 \sigma$ and $-1 \sigma$ and symmetrizing the errors. This uncertainty is found to be 1.35 GeV .
(ii) $b /$ light jet response: The calorimeter response is different for the light quark and $b$ - jets. To estimate this difference, particle jets in a $t \bar{t} l+$ jets sample were classified as $b$ - or light quark jets. Single particle response curves for both data and MC were then applied to the particle jets to predict the energy of a reconstructed jet in the calorimeter. The double ratio of jet transverse momenta in data and MC is estimated to be $1.8 \%$. We found the $b /$ light jet response systematic uncertainty by shifting the response down by $1.8 \%$ and remeasuring the top quark mass. We symmetrize this error and assign a systematic uncertainty of $\pm 0.8 \mathrm{GeV}$.


FIG. 3: Negative log likelihood distribution for data before calibration.


FIG. 4: Distribution of statistical uncertainties after correcting for the pull width and slope for $m_{\mathrm{t}}^{\mathrm{MC}}=170 \mathrm{GeV}$. Arrow indicates the measured statistical uncertainty on $m_{t}$.
(iii) Jet resolution: The jet resolution in Monte Carlo is smaller than in data. Therefore, an additional oversmearing is applied to the simulated jets. This additional oversmearing has some uncertainty. We evaluate the jet energy resolution by shifting the jet resolution by $+1 \sigma$ and $-1 \sigma$ and symmetrizing the errors. This systematic uncertainty is found to be 0.4 GeV .
(iv) Calibration uncertainty: The calibration uncertainty arises from the errors on the offset and slope of calibration curve. Using error propagation, we get an uncertainty of 0.1 GeV for the top quark mass.
(v) Template statistics: The templates have finite statistics. Local fluctuations in these templates can cause local fluctuations in the individual likelihood fits and the top quark mass. We obtain an uncertainty in $m_{\mathrm{t}}$ by varying the results of the negative likelihood fits from the data ensemble within their errors and repeating the fit to the distribution. The width of the $m_{\mathrm{t}}$ distribution provides the systematic uncertainty. It is found to be 0.35 GeV .
(vi) Initial state radiation (ISR) and final state radiation (FSR): We evaluate this systematic uncertainty by comparing Pythia with ISR and FSR parameters varied up and down [7]. After symmetrization of errors, we found this to be 0.55 GeV .
(vii) Hadronization and underlying events: We evaluate this systematic uncertainty by comparing ALPGEN + PYTHIA with HERWIG [8]. We conclude that hadronization and underlying event systematic uncertainty is 0.3 GeV .
(viii) Color reconnection: We evaluate this by comparing PYTHIA tuneACRpro [9] and tuneApro [10]. The uncertainty is found to be 0.7 GeV .
(ix) Higher order effects: We evaluate this systematic uncertainty [9] by comparing ALPGEN + PYTHIA with MC@NLO [11] + HERWIG. This is found to be 0.2 GeV .

| Source | Uncertainty (GeV) |  |  |
| :--- | :---: | :---: | :---: |
|  | $4.3 \mathrm{fb}^{-1}$ | $1 \mathrm{fb}^{-1}$ | combination |
| Statistical | $\pm 2.8$ | $\pm 4.4$ | $\pm 2.4$ |
| Jet energy scale | $\pm 1.35$ | $\pm 1.4$ | $\pm 1.4$ |
| $b$-jet energy scale | $\pm 0.8$ | $\pm 0.5$ | $\pm 0.7$ |
| Jet resolution | $\pm 0.4$ | $\pm 0.2$ | $\pm 0.3$ |
| Signal fraction | 0 | $\pm 0.1$ | 0 |
| Calibration uncertainty | $\pm 0.1$ | $\pm 0.1$ | $\pm 0.1$ |
| Template statistics | $\pm 0.35$ | $\pm 0.7$ | $\pm 0.3$ |
| ISR/FSR | $\pm 0.55$ | $\pm 0.2$ | $\pm 0.45$ |
| Hadronization and UE | $\pm 0.3$ | $\pm 0.7$ | $\pm 0.4$ |
| Color reconnection | $\pm 0.7$ | $\pm 0.7^{*}$ | $\pm 0.7$ |
| Higher order effects | $\pm 0.2$ | $\pm 0.2^{*}$ | $\pm 0.2$ |
| b fragmentation | $\pm 0.4$ | $\pm 0.4$ | $\pm 0.4$ |
| Background shape | $\pm 0.3$ | $\pm 0.3$ | $\pm 0.3$ |
| Sample dependent | 0 | $\pm 0.2$ | $\pm 0.2$ |
| Muon/track $p_{T}$ resolution | $\pm 0.2$ | $\pm 0.2$ | $\pm 0.2$ |
| Electron energy resolution | $\pm 0.2$ | $\pm 0.2$ | $\pm 0.2$ |
| Jet identification | $\pm 0.5$ | $\pm 0.5$ | $\pm 0.5$ |
| Total systematic uncertainty | $\pm 2.1$ | $\pm 2.1$ | $\pm 2.1$ |

TABLE IV: Summary of uncertainties for the Run 2 b analysis, the Run2a analysis, and their combination. Run 2a systematic uncertainties marked with * are taken from Run 2 b .

A list of all evaluated systematic uncertainties is shown in Table IV. The systematic uncertainties are dominated by jet energy scale uncertainties. The combined systematic uncertainty is $\pm 2.1 \mathrm{GeV}$.

## VIII. COMBINATION WITH THE RUN 2A DILEPTON TOP QUARK MASS MEASUREMENT.

The $\mathrm{D} \emptyset$ Collaboration has published a measurement in the dilepton channel [3] using data corresponding to an integrated luminosity of $1 \mathrm{fb}^{-1}$ from Run 2 a yielding $m_{\mathrm{t}}=174.7 \pm 4.4$ (stat.) $\pm 2.0$ (syst.) GeV. This sample is statistically uncorrelated with the sample discussed in this note. The systematic uncertainties for MC calibration and template statistics are also uncorrelated between the two measurements. All other systematic uncertainties are taken to be $100 \%$ correlated. We do not assign a sample dependent systematic uncertainty in Run 2b because of improved simulation. Color reconnection and higher order effects systematics have been estimated for the current measurement, but not for the earlier one. We have applied the newer results to the older data. Combining the two measurements [12] and accounting for correlations between uncertainties, we obtain $m_{\mathrm{t}}=173.3 \pm 2.4$ (stat.) $\pm 2.1$ (syst.) GeV .

## IX. CONCLUSION

In proton-antiproton collision data corresponding to and integrated luminosity of $5.3 \mathrm{fb}^{-1}$, we have used the neutrino weighting method to measure a top quark mass from $t \bar{t}$ events in $e \mu$ final state. We measured the top quark masss to be:

$$
m_{\mathrm{t}}=173.3 \pm 2.4 \text { (stat.) } \pm 2.1 \text { (syst.) } \mathrm{GeV}
$$

by combining the Run2b $4.3 \mathrm{fb}^{-1}$ result

$$
m_{\mathrm{t}}=172.7 \pm 2.8 \text { (stat.) } \pm 2.1 \text { (syst.) } \mathrm{GeV}
$$

with the Run2a $1.0 \mathrm{fb}^{-1}[3]$ result

$$
m_{\mathrm{t}}=173.3 \pm 2.4(\text { stat. }) \pm 2.1 \text { (syst.) GeV. }
$$

This is the most precise single measurement in the dilepton channel.
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## Measurement of the top-quark mass in $\boldsymbol{p} \overline{\boldsymbol{p}}$ collisions using events with two leptons

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#### Abstract

We present a measurement of the top-quark mass $\left(m_{t}\right)$ in $p \bar{p}$ collisions at $\sqrt{s}=1.96 \mathrm{TeV}$ using $t \bar{t}$ events with two leptons ( $e e, e \mu$, or $\mu \mu$ ) and accompanying jets in $4.3 \mathrm{fb}^{-1}$ of data collected with the D0 detector at the Fermilab Tevatron collider. We analyze the kinematically underconstrained dilepton events by integrating over their neutrino rapidity distributions. We reduce the dominant systematic uncertainties from the calibration of jet energy using a correction obtained from $t \bar{t}$ events with a final state of a single lepton plus jets. We also correct jets in simulated events to replicate the quark flavor dependence of the jet response in data. We measure $m_{t}=173.7 \pm 2.8$ (stat) $\pm 1.5$ (syst) GeV and combining with our analysis in $1 \mathrm{fb}^{-1}$ of preceding data we measure $m_{t}=174.0 \pm 2.4$ (stat) $\pm 1.4$ (syst) GeV . Taking into account statistical and systematic correlations, a combination with the D0 matrix element result from both data sets yields $m_{t}=173.9 \pm 1.9$ (stat) $\pm 1.6$ (syst) GeV .


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The masses of fundamental fermions in the standard model are generated through their interaction with a hypothesized scalar Higgs field with a strength given by a Yukawa coupling specific to each fermion species. The

[^74]Yukawa coupling of the top quark corresponds to unity within uncertainties, and this value is constrained by a measurement of the top-quark mass $\left(m_{t}\right)$. In direct searches at the LHC for the standard model Higgs boson, both the CMS and ATLAS experiments observe local excesses above the background expectations for a Higgs boson mass $\left(m_{H}\right)$ of approximately $125 \mathrm{GeV} / c^{2}[1,2]$, decaying to diboson final states. Combined results in searches from the CDF and D0 experiments at the Tevatron show evidence for events above background expectation in $b \bar{b}$ final states [3]. It is therefore important to sharpen the measurement of $m_{t}$, as its precise value, along with the mass of the $W$ boson ( $m_{W}$ ), constrains the standard model prediction for $m_{H}$ through well defined radiative corrections.

In $p \bar{p}$ collisions, top quarks $(t)$ are primarily produced in $t \bar{t}$ pairs, with each top quark decaying with $B R(t \rightarrow W b) \sim$ $100 \%$. These events yield final states with either 0,1 , or 2 leptons from decays of the two $W$ bosons. We consider the
dilepton channels ( $2 \ell$ ) that contain either electrons or muons of large transverse momentum $\left(p_{T}\right)$ and at least two jets. We analyzed such events previously $[4,5]$ using the neutrinoweighting ( $\nu \mathrm{WT}$ ) approach [6]. While the $2 \ell$ channels have low background, the small decay branching ratio into leptons means that $m_{t}$ measurements from these events remained statistically limited unlike in channels with one lepton and four or more jets ( $\ell+$ jets). This situation has changed recently (e.g., Ref. [7]). Now, dominant systematic uncertainties from jet energy calibration, which have been larger [4] in the dilepton channel compared to $\ell+$ jets, are limiting precision of the $m_{t}$ measurement. In $\ell+$ jets events, two quarks originate from $W$ boson decay and yield a dijet mass signature that permits a precise calibration of jet energies for the measurement of $m_{t}$ in $t \bar{t}$ events [8]. While this calibration has greatly improved measurements in the $\ell+$ jets channels, it has not been carried over to the calibration in other analyses. This is primarily due to differences in event topologies that can affect the details of the jet energy scale.

We present a new measurement of $m_{t}$ using the D0 detector with $4.3 \mathrm{fb}^{-1}$ of $p \bar{p}$ collider data in the $e e, e \mu$, and $\mu \mu$ final states. We improve the jet energy calibration for the accompanying jets using the energy scale from $\ell+$ jets events [9]. Our approach differs from that of Ref. [10] in that we do not use the $\ell+$ jets scale as a constraint in a combined fit of $\ell+$ jets and dilepton events. Instead, we use this constraint as a calibration, and estimate the uncertainties of transferring that calibration to the dilepton event topology. This procedure demonstrates how the calibration obtained using the dijet constraint from $m_{W}$ can be applied to different final states, and has wide applicability beyond the measurement of $m_{t}$ in $2 \ell$ events. We also employ flavordependent corrections to jet energies for the first time in a dilepton analysis that substantially reduce the uncertainties on jet energy resulting from jet flavor. The presented $m_{t}$ measurement is performed using the same data as Ref. [7], and is correlated with it as discussed below.

The D0 detector [11] is a multipurpose detector operated at the Fermilab Tevatron $p \bar{p}$ collider. The inner detector consists of coaxial cylinders and disks of silicon microstrips for track and vertex reconstruction. Eight layers of scintillating fibers arranged in doublets surround the silicon microstrip tracker and extend tracking measurements to forward pseudorapidities $\eta$ [12]. A 1.9 T solenoid produces a magnetic field for the tracking detectors. Uranium-liquid argon calorimeters surround the tracking volume and perform both electromagnetic and hadronic shower energy measurements. Thin scintillation intercryostat detectors sample showers in the region between the central and end calorimeters. Three layers of proportional drift tubes and scintillation counters reside outside the calorimetry, with 1.8 T toroids that provide muon identification and independent measurement of muon momenta.

We simulate $t \bar{t}$ events using Monte Carlo (MC) samples for $140 \mathrm{GeV}<m_{t}<200 \mathrm{GeV}$ using the ALPGEN
generator [13] and PYTHIA [14] for parton fragmentation. Backgrounds originate from $Z / \gamma^{*} \rightarrow 2 \ell+$ jets and $W W / W Z / Z Z \rightarrow 2 \ell+$ jets production. For the former, we use ALPGEN combined with PYTHIA, while diboson backgrounds are simulated entirely with PYTHIA. We pass all MC events through a full detector simulation based on GEANT [15]. Backgrounds from instrumental effects that result in misidentified leptons are modeled using data.

We use single and two-lepton triggers to select events for this analysis. Data and simulated events are reconstructed to provide the momenta of tracks, jets, and lepton candidates. Charged leptons are required to be isolated from other calorimeter energy deposits, and to have an associated track in the inner detector. Calorimeter and tracking information are combined to identify electrons. Track parameters in the muon and inner detector system are used to identify muons. We reconstruct jets with an iterative, midpoint cone algorithm with radius $\mathcal{R}_{\text {cone }}=0.5$ [16]. Jets are calibrated with the standard D0 jet energy correction which is derived from data [17]. The method corrects the measured jet energy to the value obtained by applying the reconstruction cone algorithm to particles from jet fragmentation before they interact with the detector. We establish the efficacy of the method in the MC, where we compare the measured jet and the jet reconstructed from fragmentation particles. The jets in data and MC are calibrated independently so that their relative response is close to unity. This corrects for detector response, energy deposited outside of the jet cone, electronics noise, and pileup. The largest correction compensates for the detector response, and is extracted using $\gamma+$ jet events in data and MC. We also correct jets for the $p_{T}$ of any embedded muon and that of the associated neutrino. We initially apply this standard calibration [17] because it provides detailed $p_{T}$ and $\eta$ dependent corrections. It also provides distinct corrections to jets and the imbalance in event transverse momentum $\left(\boldsymbol{E}_{T}\right)$ because several components (e.g., noise and out-of-cone effects) result from the jet reconstruction algorithm rather than any undetected energy. In the $p_{T}$ range of jets found in $t \bar{t}$ events, the uncertainty of the standard D0 jet energy calibration averages $2 \%$, and is dominated by systematics. Because the flavor dependence of jet energy calibration can yield one of the largest systematic uncertainties on our measurement [4], we have improved our analysis by accounting for this dependence. We use responses of single particles from data and MC to determine the energy scale for different jet flavors. We correct MC jets by the ratio of data response to MC response according to their flavor to ensure that the MC reflects the flavor dependence in data, as in Ref. [9]. We calculate $\mathscr{L}_{T}$ as the negative of the vector sum of all transverse components of calorimeter cell energies and muon track momenta, corrected for the response to electrons and jets.

Events are selected to have two leptons ( $e e, e \mu, \mu \mu)$ and two or more jets. The leptons must have $p_{T}>15 \mathrm{GeV}$
and the jets must have $p_{T}>20 \mathrm{GeV}$. Electrons and jets are required to satisfy $|\eta|<2.5$, while muons must have $|\eta|<2$. We further require $\mathscr{E}_{T}>40 \mathrm{GeV}$ in the $\mu \mu$ channel. The $e \mu$ events must satisfy $H_{T}>120 \mathrm{GeV}$, where $H_{T}$ is defined to be the sum of the $p_{T}$ 's of jets and the leading lepton. In $\mu \mu$ and $e e$ events, we also require $\mathbb{E}_{T}$ to be significantly larger than typical values found in the distribution from $Z$ boson events. These and all other selections are detailed in Ref. [18]. We observe 50,198 , and 84 events with expected background yields of $10.4,28.1$, and 31.0 events in the $e e, e \mu$, and $\mu \mu$ channels, respectively.

In $\ell+$ jets events, one $W$ boson decays to two quarks that fragment to jets. The invariant mass of this jet pair can be used to improve the calibration for all jets in these events. Complications arise because the four jets in the $\ell+$ jets events can be incorrectly assigned to the initial four quarks. Energy from different partons is also mixed in the same jet due to a high jet multiplicity. Observed jet energies are also affected by color flow effects, which are different for the $b$-quark jets and for jets from the decay of color singlet $W$ bosons. These attributes are specific to a particular event topology such as $\ell+$ jets. Nevertheless, a scale factor based on the dijet invariant mass that is correlated with $m_{W}$ can be extracted. The most recent analysis of this kind by D0 used $2.6 \mathrm{fb}^{-1}$ of data and obtained a calibration factor of $1.013 \pm 0.008$ (stat) [9]. The uncertainty of $0.8 \%$ is smaller than that of the standard jet energy correction and will decrease with additional data. There are additional systematic effects on this energy scale that one must account for when applying it to $b$-quark jets in the $\ell+$ jets analysis. These also affect our analysis, and we similarly evaluate the flavor dependence and residual energy scale systematic uncertainties directly on the measured $m_{t}$ to avoid double counting. These are quoted in Table II and discussed below. Beyond this, we have the possible difference between $b$-quark jets in dilepton events and $b$-quark jets in $\ell+$ jets events and the effect of using a calibration based on a subset of the total data, each of which we discuss now in detail.

The event topology is different in $2 \ell$ and $\ell+$ jets events. This has prevented significant progress in reducing the large standard jet energy scale uncertainties in dilepton analyses. To overcome this challenge and carry over the $\ell+$ jets calibration, we must account for the possibility that the energy scale of the $b$-quark jets in the two channels can differ. We calculate the energy scale $R^{2 \ell}$ for $b$-quark jets in the dilepton sample using responses for single particles that fall within the reconstructed jet cone. This is done by scaling single particle responses in MC to reproduce the energy response of jets in data [19], giving $R_{\text {data }}^{2 \ell}$, and using particle responses from MC, giving $R_{\mathrm{MC}}^{2 \ell}$. We calculate the ratio of these two responses in the dilepton channel and the analogous ratio for $b$-quark jets in the $\ell+$ jets sample. The corresponding double ratio

$$
\begin{equation*}
\mathcal{R}_{2 \ell}^{b}\left(p_{T}^{b}\right)=\frac{R_{\text {data }}^{2 \ell}\left(p_{T}^{b}\right) / R_{\mathrm{MC}}^{2 \ell}\left(p_{T}^{b}\right)}{R_{\text {data }}^{\ell+\text { jets }}\left(p_{T}^{b}\right) / R_{\mathrm{MC}}^{\ell+\text { jets }}\left(p_{T}^{b}\right)} \tag{1}
\end{equation*}
$$

varies between 1.001 and 1.003 depending on $b$-quark jet $p_{T}, p_{T}^{b}$. The multiplicity of particles in $b$-quark jets in $\ell+$ jets events at the MC generator level is, after application of the offline jet algorithm, a few percent higher than in the dilepton sample, which is a sufficiently large difference to account for the observed value of $\mathcal{R}_{2 \ell}^{b}$. We therefore take $0.3 \%$, the maximum excursion of $\mathcal{R}_{2 \ell}^{b}$ from unity, as a systematic uncertainty on carrying over the $\ell+$ jets scale to the jets in our dilepton sample. The $\ell+$ jets scale is applied as a direct correction to the standard calibration.

The jet energy scale calibration obtained in Ref. [9] is based on a subset of the data, and we must therefore estimate the effect of using the calibration on a larger data set. The instantaneous luminosity of the dilepton sample is higher on average. We reweight the distribution of the number of primary vertices in the $\ell+$ jets sample to match the distribution in the $4.3 \mathrm{fb}^{-1} \ell+$ jets data and recalculate the $\ell+$ jets energy scale. This produces a negligible effect. To account for a possible shift in the energy scale of the liquid argon calorimeter, we apply a correction derived from $4.3 \mathrm{fb}^{-1}$ rather than $2.6 \mathrm{fb}^{-1}$, and this yields a $0.7 \%$ shift in jet energy scale. From these studies, we obtain a total uncertainty on the $\ell+$ jets energy scale as applied to our analysis as the sum in quadrature of the statistical uncertainty $(0.8 \%), \mathcal{R}_{2 \ell}^{b}(0.3 \%)$, and the calorimeter calibration ( $0.7 \%$ ). This yields a $1.1 \%$ uncertainty for applying the $\ell+$ jets energy scale.

The consequence of two neutrinos in dilepton events is an underconstrained kinematics. We employ the $\nu \mathrm{WT}$ technique to extract $m_{t}$ [6] due to its weak sensitivity to the modeling details of $t \bar{t}$ events. We integrate over the $\eta$ distributions predicted for both neutrinos, solve the event kinematics, and calculate $\mathbb{Z}_{T}$ from the neutrino momentum solutions. The expected neutrino $\eta$ distribution in the dilepton channel is symmetric around $\eta=0$ and found to be well described by a Gaussian distribution. The width of the distribution decreases gradually with increasing $m_{t}$ (i.e., as the neutrinos become more central). Hence, we model the neutrino $\eta$ distributions with a Gaussian probability distribution using a width parameterized as a linear function of $m_{t}$. Several more sophisticated parametrizations were tested, but provided negligible improvement in expected precision in pseudoexperiments. By comparing the calculated $\mathscr{E}_{T}$ to the measured $\mathscr{E}_{T}$ for each event, we calculate a weight for a given choice of $m_{t}$. For each neutrino rapidity sampling, we sum the weights calculated from all combinations of neutrino momentum solutions and jet assignments. We therefore arrive at a distribution of relative weight for a range of $m_{t}$ for each event. We found in Ref. [4] that most of the statistical sensitivity to $m_{t}$ is obtained from the first two moments of this weight distribution, the mean $\left(\mu_{w}\right)$ and $\mathrm{rms}\left(\sigma_{w}\right)$. A coarse
granularity of our sampling of the $\eta$ distribution causes these moments to be unstable. To reduce this variation, we have increased the sampling for this integration by an order of magnitude relative to our previous analysis [4]. This improves the expected statistical uncertainty on $m_{t}$ by $4 \%$. Requiring the integral of this distribution to be nonzero excludes events with a measured $\mathbb{E}_{T}$ that is incompatible with coming from neutrinos from $t \bar{t}$ decay. This introduces a small inefficiency for the $t \bar{t}$ signal and reduces the background contamination in the final sample. Our final kinematically reconstructed data sample consists of 49,190 , and 80 events in the $e e, e \mu$, and $\mu \mu$ channels, respectively.

Probability distributions for $\mu_{w}$ and $\sigma_{w}$ are constructed for background in each channel. Each background component is normalized to its expected event yield. We generate distributions of $t \bar{t}$ signal probability as a function of $\mu_{w}$, $\sigma_{w}$, and $m_{t}$. We use a binning that provides the minimum expected statistical uncertainty, as checked in pseudoexperiments. We perform a binned maximum likelihood fit to the probability distributions, fixing the total signal and background yields expected in our data. The signal is normalized to the cross section calculated for $t \bar{t}$ production [20], evaluated at $m_{t}=172.5 \mathrm{GeV}$. For all measurements, we obtain a likelihood $(L)$ vs $m_{t}$. We fit a parabola to the dependence of $-\ln L$ vs $m_{t}$, and the fitted mass $m_{t}^{\text {fit }}$ is defined as the lowest point of the parabola. Point-to-point fluctuations mean that the initial placement of the window may result in a nonconvergent fit. We therefore iterate the fit around the current fit minimum. This results in a significant improvement in fitting efficiency, particularly in the dimuon channel. The final $-\ln L$ vs $m_{t}$ for data is shown in Fig. 1. The statistical uncertainty for each measurement is taken as the half-width of the parabola at 0.5 units in $-\ln L$ above the minimum at $m_{t}^{\mathrm{fit}}$.

The above procedure is followed for the extraction of $m_{t}$ from data and is used to calibrate the result as follows. We construct pseudoexperiments from signal and background MC samples according to their expected yields and allow fluctuations in each such that the total equals the number of observed events. We perform 1000 pseudoexperiments for


FIG. 1. $\ln L$ as a function of $m_{t}$ for the combined $e e, e \mu$, and $\mu \mu$ channels. A parabolic fit is shown near the minimum value in $m_{t}$.
each channel, and measure $m_{t}^{\text {fit }}$ in each. A linear fit of $m_{t}^{\text {fit }}$ vs the input $m_{t}$ provides a calibration for our method. We also calculate the pull width of the average estimated statistical uncertainty vs the rms of $m_{t}^{\text {fit }}$ values. The resulting slopes, offsets, and pull widths are given in Table I. The $m_{t}^{\text {fit }}$ and estimated statistical uncertainty are corrected with these parameters. We obtain a calibrated mass measurement for the $4.3 \mathrm{fb}^{-1}$ sample in the $e e, e \mu$, and $\mu \mu$ channels.

The largest systematic uncertainties are associated with the jet calibration. We change the $\ell+$ jets energy scale factor by $\pm 1.1 \%$, and perform our analysis to obtain a systematic uncertainty on $m_{t}$ of 0.9 GeV . The result of the $\ell+$ jets analysis is a single scale factor averaged over all jet $p_{T}$ 's that are utilized in the dijet mass, i.e., dominated by light quark jets from $W$ boson decay. As in Ref. [9], we estimate an uncertainty due to the difference in $p_{T}$ distributions of $b$-quark jets, in our case in dilepton events, vs the calibrating jets from the $W \rightarrow j j$ sample. To estimate an uncertainty from this difference, we treat the $p_{T}$ and $\eta$ dependence of the uncertainty in the standard jet energy scale as a possible dependence of the residual energy scale following the calibration to $\ell+$ jets. We calculate the average of the energy scale uncertainty for jets in the $W \rightarrow j j$ sample. For each jet in the dilepton sample, we apply a shift corresponding to the difference between its uncertainty in energy scale and the $W \rightarrow j j$ sample's average uncertainty in energy scale. Propagating this difference through the mass analysis yields a 0.3 GeV uncertainty on $m_{t}$.

The flavor-dependent jet energy corrections described earlier provide MC-based mass templates that accurately reflect the data. As in [9], we propagate the uncertainty in these corrections and obtain a systematic uncertainty on $m_{t}$ of 0.5 GeV . The uncertainties due to flavor dependence and residual scale together with the uncertainty originating from the carry over of the jet energy scale from the $\ell+$ jets sample account for the difference between $b$-quark jets in dilepton events and jets from $W \rightarrow j j$ in $\ell+$ jets events.

We evaluate the effect of our uncertainty in modeling initial state radiation (ISR) and final state radiation (FSR) by comparing two PYTHIA samples having identical values of generated $m_{t}$ but different input parameters taken from a CDF study [21] corresponding to an increased or decreased amount of ISR/FSR. Color reconnection uncertainties are estimated by comparing the analysis with PYTHIA tune Apro and PYTHIA tune ACpro using [22]. Higher order

TABLE I. Parameters used to calibrate $m_{t}^{\mathrm{fit}}$ in the analysis of $e e, e \mu$, and $\mu \mu$ channels and their combination.

| Channel | Slope | Offset $[\mathrm{GeV}]$ | Pull width |
| :--- | :---: | :---: | :---: |
| $e e$ | $0.976 \pm 0.014$ | $0.03 \pm 0.16$ | $1.01 \pm 0.01$ |
| $e \mu$ | $0.973 \pm 0.012$ | $0.43 \pm 0.14$ | $1.03 \pm 0.01$ |
| $\mu \mu$ | $1.038 \pm 0.022$ | $0.49 \pm 0.23$ | $1.06 \pm 0.03$ |

TABLE II. Estimated systematic uncertainties on $m_{t}$ for the combined dilepton measurement in $4.3 \mathrm{fb}^{-1}$.

| Source | Uncertainty $(\mathrm{GeV})$ |
| :--- | :---: |
| Jet energy calibration |  |
| Overall scale | 0.9 |
| Flavor dependence | 0.5 |
| Residual scale | 0.3 |
| Signal modeling |  |
| ISR/FSR | 0.4 |
| Color reconnection | 0.5 |
| Higher order effects | 0.6 |
| $b$ quark fragmentation | 0.1 |
| Parton distribution function uncertainty | 0.5 |
| Object reconstruction |  |
| Muon $p_{T}$ resolution | 0.2 |
| Electron energy scale | 0.2 |
| Muon $p_{T}$ scale | 0.2 |
| Jet resolution | 0.3 |
| Jet identification | 0.3 |
| Method |  |
| Calibration | 0.1 |
| Template statistics | 0.5 |
| Signal fraction | 0.2 |
| Total systematic uncertainty | 1.5 |

QCD evolution is estimated by comparing ALPGEN configured with PYTHIA to MC@NLO with HERWIG [23] and this accounts for the uncertainty due to underlying event as well. To estimate sensitivity to uncertainties in the parton distribution functions, we use CTEQ6M, and employ the method described in Ref. [24].

We modify the jet energy resolution in MC events to reflect the resolution in data. We evaluate the effect of an uncertainty in this procedure on the extraction of $m_{t}$ by shifting the jet resolution by 1 standard deviation. We treat the electron and muon energy and momentum scales similarly and shift their calibrations within their uncertainties.

Pseudoexperiments are used similarly to account for the uncertainty in the method that arises from the uncertainties on the offset and slope in the calibration of the fitted $m_{t}$. We estimate the uncertainty due to the statistics employed in our templates of the $t \bar{t}$ probability distributions. We construct 1000 new templates, for both signal and background,
and vary their bin contents within their Gaussian uncertainties. With these templates, we obtain 1000 new measurements from data and quote the rms of these values as a systematic uncertainty. We assign a systematic uncertainty on the signal fraction by shifting the background contributions in pseudoexperiments within their total uncertainty.

We combine measurements in the three dilepton channels using the method of "best linear unbiased estimator" [25]. We calculate each systematic uncertainty for the combined result, as given in Table II, according to its correlation among channels. The resulting measurement gives $m_{t}=173.7 \pm 2.8$ (stat) $\pm 1.5$ (syst) GeV .

We combine this measurement with D0's measurement in the preceding $1 \mathrm{fb}^{-1}$ of data using the $\nu \mathrm{WT}$ and matrix weighting methods [4]. Some uncertainties evaluated in the $4.3 \mathrm{fb}^{-1}$ sample are not available for the $1.0 \mathrm{fb}^{-1}$ sample. We include the new uncertainties in the result from the previous analysis. We consider statistical uncertainties, as well as the following systematic uncertainties to be uncorrelated: calibration of method, template statistics, overall jet energy scale, and flavor dependence. We consider all other uncertainties to be fully correlated. The combined measurement yields $m_{t}=174.0 \pm 2.4$ (stat) $\pm 1.4$ (syst) GeV . This is consistent with measurements in other channels, and is the most precise single $m_{t}$ measurement in the dilepton channel to date. We have also improved the precision by combining the $\nu \mathrm{WT}$ results with the results of Ref. [7]. The statistical correlation of these two measurements is approximately $60 \%$, calculated from pseudoexperiments. Accounting for this correlation, and correlations appropriate to each source of systematic uncertainty, we obtain $m_{t}=173.9 \pm$ 1.9 (stat) $\pm 1.6$ (syst) GeV .

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# Combination of the top-quark mass measurements from the Tevatron collider 

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#### Abstract

The top quark is the heaviest known elementary particle, with a mass about 40 times larger than the mass of its isospin partner, the bottom quark. It decays almost $100 \%$ of the time to a $W$ boson and a bottom quark. Using top-antitop pairs at the Tevatron proton-antiproton collider, the CDF and D0 Collaborations have measured the top quark's mass in different final states for integrated luminosities of up to $5.8 \mathrm{fb}^{-1}$. This paper reports on a combination of these measurements that results in a more precise value of the mass than any individual decay channel can provide. It describes the treatment of the systematic uncertainties and their correlations. The mass value determined is $173.18 \pm 0.56$ (stat) $\pm 0.75$ (syst) GeV or $173.18 \pm 0.94 \mathrm{GeV}$, which has a precision of $\pm 0.54 \%$, making this the most precise determination of the top-quark mass.


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## I. INTRODUCTION

## A. The top quark

The standard model (SM) of particle physics describes the elementary particles and their interactions. The top quark $(t)$ has a special place in the hierarchy of particles because it is far more massive than any of the other fundamental objects. It is the up-type quark, partnered with the down-type bottom quark ( $b$ ), forming the third generation of quarks that was predicted by Kobayashi and Maskawa in 1973 [1] to accommodate $C P$ violation in neutral kaon decays [2]. At particle colliders the top quark is produced mainly in top-antitop $(t \bar{t})$ pairs. The first evidence of top-quark production was reported by the CDF Collaboration [3], and the top quark was first observed in this production mode by the CDF [4] and D0 [5] Collaborations at the Tevatron proton-antiproton collider. Since then, great efforts have been focused on measuring its properties with ever higher precision. In addition to its large mass $\left(m_{t}\right)$, the top quark is also singular because it decays before it can hadronize: there are no mesons or baryons containing valence top quarks. The top quark decays almost exclusively to a $W$ boson and a $b$ quark, with the fraction determined by the near-unity value of the Cabibbo-Kobayashi-Maskawa (CKM) quark mixing matrix [1,6] element $V_{t b}(\approx 0.9992)$ [7]. Its other decays are limited by the small values of $V_{t s} \approx 0.0387$ and $V_{t d} \approx$ 0.0084 [7], assuming three-family unitarity of the CKM matrix. The $W$ boson decays to a charged lepton and its
associated neutrino, or to a quark-antiquark pair, and the final states of $t \bar{t}$ events are thus characterized as follows: "lepton + jets" $\left(t \bar{t} \rightarrow \ell^{+} \nu b q \bar{q}^{\prime} \bar{b}\right.$ and $\left.\bar{q} q^{\prime} b \ell^{-} \bar{\nu} \bar{b}\right)$; "alljets" $\left(t \bar{t} \rightarrow q \bar{q}^{\prime} b \bar{q} q^{\prime} \bar{b}\right)$, and "dileptons" $\left(t \bar{t} \rightarrow \ell^{+} \nu b \ell^{-} \bar{\nu} \bar{b}\right)$. In this notation the charged lepton $\ell$ represents an electron or muon, and $q$ is a first- or second-generation quark. The $W$ boson also decays to a $\tau$ lepton and a $\tau$ neutrino. If $\tau$ decays to an electron or muon, the event contributes to the lepton categories, and if the $\tau$ decays into hadrons, it contributes to the lepton + jets or alljets categories. A fourth category labeled " $\dot{E}_{T}+$ jets" is used to measure $m_{t}$ when there are jets and a large imbalance in transverse momentum in the event $\left(\mathbb{E}_{T}\right)$, but no identified lepton. It comprises $t \bar{t} \rightarrow \tau^{+} \nu b \tau^{-} \bar{\nu} \bar{b}, \tau^{+} \nu b q \bar{q}^{\prime} \bar{b}$, and $\bar{q} q^{\prime} b \tau^{-} \bar{\nu} \bar{b}$ final states, accounting for $40 \%$ of the $t \bar{t}$ signal events in the $\mathscr{E}_{T}+$ jets category, or $\ell^{+} \nu b q \bar{q}^{\prime} \bar{b}, \bar{q} q^{\prime} b \ell^{-} \bar{\nu} \bar{b}$, where the electron or muon are not reconstructed, accounting for $60 \%$ of the $t \bar{t}$ signal in this category. Additional contributions to $\mathscr{E}_{T}$ arise from the neutrino(s) produced in $\tau$ decays.

In dilepton events, there are typically two jets from the two $b$ quarks, one from each top-quark decay. In lepton + jets events, there are typically four jets, including two $b$ jets and two light-quark jets from $W$-boson decay. Alljets events most often contain six jets, the two $b$ jets and four light-quark jets. The $\mathbb{E}_{T}+$ jets events usually have four or five jets. Additional gluon or quark jets can arise owing to radiation from initial or final-state colored particles, including the top quarks. About $23 \%$ of the $t \bar{t}$ events have an extra jet with sufficient energy to pass the selection criteria,


FIG. 1 (color online). Examples of tree Feynman diagrams for $t \bar{t}$ production. At the Tevatron collider, the $q \bar{q}$ channel contributes $81 \%$ to the total $t \bar{t}$ inclusive cross section and the $g g$ channel the remaining $19 \%$ [69,96].


FIG. 2 (color online). Leading-order Feynman diagram for $t \bar{t}$ decay. The dilepton modes ( $e e, e \mu, \mu \mu$ ) have a combined branching fraction of $\approx 4 \%$, the electron + jets and muon + jets modes combined correspond to $\approx 30 \%$, and the alljets mode has a branching fraction of $\approx 46 \%$. The $\tau$ modes are shared among the $\mathscr{L}_{T}+$ jets and the other channels in the analyses.
and about $5 \%$ of the events have two additional jets. These extra jets complicate the measurement of $m_{t}$ and degrade its resolution. Figure 1 illustrates leading-order (LO) production of $t \bar{t}$ events at the Fermilab Tevatron Collider, and Fig. 2 shows the relevant $t \bar{t}$ decay modes.

## B. Top-quark mass origin and definitions

One of the fundamental properties of an elementary particle is its mass. In the SM, fermions acquire mass through interactions with the Higgs field [8]. Absolute values of these masses are not predicted by the SM. In theoretical calculations, a particle's mass can be defined in more than one way, and it depends on how higher-order terms in perturbative quantum chromodynamics (QCD) calculations are renormalized. In the modified minimal subtraction scheme ( $\overline{\mathrm{MS}}$ ), for example, the mass definition reflects short-distance effects, whereas in the pole-mass scheme the mass definition reflects long-distance effects [9]. The concept of the pole mass is not well defined since color confinement does not provide $S$-matrix poles at $m=m_{t}$ [10]. Direct mass measurements that are inputs to the combination described in this paper rely on Monte Carlo (MC) generators to extract $m_{t}$. Hence the measured mass corresponds in fact to the mass parameter in the MC. Work is proceeding to address the exact differ-
ence between the measured mass and the pole mass, as presented, for example, in Appendix C of Ref. [11]. One alternative way to address this problem is to extract $m_{t}$ from a measurement of the $t \bar{t}$ cross section [12]. The D0 Collaboration has recently shown that the directly measured mass of the top quark is closer to the pole mass extracted from a measurement of the $t \bar{t}$ cross section than to an $\overline{\mathrm{MS}}$ mass extracted in a similar way [12]. Hence, within the precision of theory and data, the directly measured $m_{t}$ is best interpreted as the top-quark pole mass.
$C P T$ invariance predicts that a particle and its antiparticle partner have the same mass. This has been checked for the top quark by the $\mathrm{D} 0, \mathrm{CDF}$, and CMS Collaborations, and the masses are found to hold within the measurement uncertainties, with $\Delta m_{t}=m_{t}-m_{\bar{t}}=0.84 \pm 1.87 \mathrm{GeV}$ [13], $\Delta m_{t}=-3.3 \pm 1.7 \mathrm{GeV}$ [14], and $\Delta m_{t}=-0.44 \pm$ 0.53 GeV [15], respectively. Thus, the top-quark mass combination in this paper assumes $m_{t}=m_{\bar{t}}$.

## C. Predictions based on the top-quark mass

The internal consistency of the SM can be tested by using different observables to predict the values of others and then to compare the expectations with their measured values. For example, the relation between the mass of the $W$ boson $\left(M_{W}\right)$ and $\sin ^{2} \theta_{W}$ (the electroweak mixing angle) includes higher-order radiative corrections involving $m_{t}$; hence the smaller the uncertainty on the measured $m_{t}$, the stronger is the test of consistency.

Since 1997, the LEP Electroweak Working Group has used the observed top-quark and the $W$ boson masses and other precision electroweak variables to extract constraints on the Higgs boson mass ( $M_{H}$ ) in the SM [16]. This has been extended to the minimal supersymmetric standard model [17], and the GFITTER Collaboration has applied the technique to set limits on a wide variety of theories beyond the SM [18]. Figure 3(a) shows the combined constraint attributable to $M_{W}$ and $m_{t}$ (as of March 2012) on the Higgs boson mass. Figure 3(b) shows the constraint from $M_{W}$ and $m_{t}$ separately (as of March 2012) on the Higgs boson mass, and a global constraint originating from all the other electroweak variables, showing the importance of the $M_{W}$ and $m_{t}$ variables to constrain the Higgs boson mass.

## D. History of measurement of $\boldsymbol{m}_{\boldsymbol{t}}$

Before 1995, global fits to electroweak data from the CERN and SLAC $e^{+} e^{-}$colliders (LEP and SLC) and from other experiments produced estimates of $m_{t}$ that ranged from $\approx 90 \mathrm{GeV}$ to $\approx 190 \mathrm{GeV}$ [19]. At the time of the first observation of the top quark in 1995, the fits indicated a mass close to the current Tevatron value of $m_{t}$, but with an uncertainty of $\approx \pm 10 \%$ and an assumption of 300 GeV mass of the Higgs boson [20]. CDF measured $m_{t}=176 \pm$ 8 (stat) $\pm 10$ (syst) GeV [4] (total uncertainty of $7 \%$ ) and


FIG. 3 (color online). (a) Constraints from LEP and Tevatron measurements of $M_{W}$ and $m_{t}$ (Tevatron only) on $M_{H}$ within the SM. The regions in the mass of the Higgs boson still allowed after the direct searches at LEP, Tevatron, and LHC are also shown. (b) From Ref. [18], the large countors (blue) indicate the constraints on the Higgs boson, from global fits to electroweak data without including the direct measurements of $M_{W}$ and $m_{t}$ from the Tevatron.

D0 measured $m_{t}=199_{-21}^{+19}($ stat $) \pm 22$ (syst) GeV [5] (total uncertainty of $15 \%$ ).

Since then, the CDF and D0 Collaborations have developed many novel measurement techniques and published nearly 50 journal papers on their measurements of $m_{t}$. Recently, the CMS Collaboration at the Large Hadron Collider (LHC) published a measurement using 102 dilepton events [21] and finds $m_{t}=175.5 \pm 4.6$ (stat) $\pm$ 4.6 (syst) GeV (total uncertainty of $3.7 \%$ ). The ATLAS Collaboration at the LHC has submitted a measurement of $m_{t}=174.5 \pm 0.6 \pm 2.3 \mathrm{GeV}$ (total uncertainty of $1.4 \%$ ) using nearly 12,000 lepton + jets events [22]. The most precise measurements from the Tevatron in a single decay channel use lepton + jets events, a matrix-element
method as introduced in Ref. [23], and an in situ calibration of the jet energy scale. CDF's matrix-element measurement [24] uses $5.6 \mathrm{fb}^{-1}$ of integrated luminosity to find $m_{t}=173.00 \pm 0.65$ (stat) $\pm 1.06$ (syst) GeV (total uncertainty of $0.72 \%$ ). D0's measurement [25] uses $3.6 \mathrm{fb}^{-1}$ of integrated luminosity to obtain $m_{t}=174.94 \pm 0.83$ (stat) $\pm$ 1.24 (syst) GeV (total uncertainty of $0.85 \%$ ). Figure 4 shows the publication history of the direct measurements of $m_{t}$ at the Tevatron.

## E. Overview of mass measurements

This paper reports on the combination of previously published measurements of $m_{t}$. Details of the analyses are therefore not repeated as this information is available in recent reviews [26], as well as in the publications of each of the results. We will, however, summarize the basic techniques used for the measurements.

The cross section for $t \bar{t}$ production in proton-antiproton $(p \bar{p})$ interactions at 1.96 TeV is $\approx 7.2 \mathrm{pb}[27,28]$. The mean transverse momentum ( $p_{T}$ ) of the $t \bar{t}$ system at parton level is $\approx 20 \mathrm{GeV}$, which is attributed to initial-state radiation (i.e., gluon emission). The mean transverse momentum of the top quarks at parton level is $\approx 95 \mathrm{GeV}$ [29]. Top quarks have a lifetime of $\approx 0.3 \times 10^{-24} \mathrm{~s}[30,31]$, which is an order of magnitude smaller than the time scale for parton evolution and hadronization. Hence, when top quarks decay, they transfer their kinematic characteristics to the $W$ boson and $b$ quark, and the measured energymomentum four-vectors of the final-state particles can be used to reconstruct the mass of the top quark, except for the presence of initial or final-state radiation.

In alljets events, the four-vector of every jet emerging from quarks can be reconstructed, but neutrinos emitted in semileptonic decays of $b$ quarks and jet energy resolution effects will lead to lost energy. In lepton + jets events, the momentum of the neutrino from the $W \rightarrow \ell \nu_{\ell}$ decay is not detected. The transverse component can be inferred from the negative of the vector sum of all transverse momenta of particles detected in the calorimeter and muon detectors. We estimate the longitudinal momentum of $\nu_{\ell}$ by constraining the mass of the charged lepton and neutrino system to the world average value of $M_{W}$ [7]. We also use $M_{W}$ to choose the two light jets from $W \rightarrow q \bar{q}^{\prime}$ decay, and we use that information for an in situ calibration of jet energies. In dilepton events, the analysis is more complicated because there are two final-state neutrinos from the leptonic decays of both $W$ bosons. Therefore, the longitudinal and transverse-momentum components of the neutrinos cannot be determined without the application of more sophisticated tools. These involve assuming a value for $m_{t}$ to solve the event kinematics and assigning a weight to each $m_{t}$ hypothesis to determine the most likely value of $m_{t}$ consistent with the hypothesis that the event is a $t \bar{t}$ event.

A major issue in $t \bar{t}$ final-state reconstruction is the correct mapping of the reconstructed objects to the partons


FIG. 4 (color online). The CDF and D0 published direct measurements of the top-quark mass as a function of time.
from the decays of the top quark and $W$ boson. The problem arises because often the jet charge and flavor cannot be uniquely determined. This creates combinatorial ambiguities in the $t \bar{t}$ event reconstruction that vary from 90 possible jet-to-parton assignments for the alljets final state to 2 in the dilepton channel. In the lepton + jets and dilepton final states, additional ambiguities may arise from multiple kinematical solutions for the longitudinal component of the neutrino momentum.

Two methods are used to measure the value of $m_{t}$. In the first method, the reconstructed mass distribution in data, or a variable correlated with $m_{t}$, such as the decay length of the $B$ hadron or the transverse momentum of a lepton, is compared to template distributions composed of contributions from background and simulation of $t \bar{t}$ events. One template is used to represent background and another for each putative value of $m_{t}$. The second method uses event probabilities based on the LO matrix element for the production of $t \bar{t}$. For each event, a probability is calculated as a function of $m_{t}$ that this event is from $t \bar{t}$ production, as based on the corresponding production and decay matrix element. Detector resolution is taken into account in the calculation of these probabilities through transfer functions that correlate parton-level energies and their measured values. The value of $m_{t}$ is then extracted from the joint probability calculated for all selected events, based on the probability for signal and background (also defined through its matrix element). This method produces the most accurate results, but the computations are time consuming.

## F. Combination overview

This paper describes the combination of statistically independent top-quark mass measurements from the

Fermilab Tevatron Collider. Measurements are independent if they are based on different data sets, e.g., from CDF and from D0, or from Tevatron Run I (1992-1996) and Run II (2001-2011). They are also independent within one data set if the event selections are designed to be exclusive; i.e., no event can pass more than one category of selections. At times, more than one measurement is published using the same data and decay channel. In this situation, the result with smallest overall uncertainty is chosen for the combination. Twelve measurements are used in the combination described here, eight from the CDF collaboration and four from D0. These comprise five lepton + jets measurements (CDF and D0, Run II and Run I, and a CDF Run II result based on the decay length of $B$ hadrons); two alljets measurements (CDF Run II and Run I); four dilepton measurements (CDF and D0, Run II and Run I); and a $\mathscr{E}_{T}+$ jets measurement (CDF Run II). We combine these measurements using an analytic method called the best linear unbiased estimator (BLUE) [32-34]. This technique forms a linear combination of the separate unbiased mass measurements to produce the best estimate of $m_{t}$ with the smallest uncertainty. This procedure follows a series of 11 such mass combinations presented in [35-45], updated each year since 2004 as new measurements of $m_{t}$ became available. The combination presented here is the first to be published in a peer-reviewed journal.

## II. INPUTS TO THE COMBINATION

## A. The independent mass measurements

The mass measurements included in the combination are shown in Table I [24,25,46-55]. These 12 channels are chosen because they are statistically independent, which

TABLE I. Top-quark mass measurements used as input to determine the combined value of $m_{t}$ from the Tevatron and the combined result.

| Decay channel or method | Tevatron period | Experiment | Integrated luminosity $\left[\mathrm{fb}^{-1}\right]$ | Number of events | Background [\%] | $m_{t}[\mathrm{GeV}]$ | Uncertainty on $m_{t}$ [\%] | Reference |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Lepton + jets | Run II | CDF | 5.6 | 1087 | 17 | $173.00 \pm 0.65 \pm 1.06$ | 0.72 | [24] |
| Lepton + jets | Run II | D0 | 3.6 | 615 | 27 | $174.94 \pm 0.83 \pm 1.24$ | 0.85 | [25] |
| Lepton + jets | Run I | CDF | 0.1 | 76 | 54 | $176.1 \pm 5.1 \pm 5.3$ | 4.2 | [46] |
| Lepton + jets | Run I | D0 | 0.1 | 22 | 22 | $180.1 \pm 3.6 \pm 3.9$ | 2.9 | [47] |
| Alljets | Run II | CDF | 5.8 | 2856 | 71 | $172.47 \pm 1.43 \pm 1.40$ | 1.2 | [48] |
| Alljets | Run I | CDF | 0.1 | 136 | 79 | $186.0 \pm 10.0 \pm 5.7$ | 6.2 | [49] |
| Dileptons | Run II | CDF | 5.6 | 392 | 23 | $170.28 \pm 1.95 \pm 3.13$ | 2.2 | [50] |
| Dileptons | Run II | D0 | 5.3 | 415 | 21 | $174.00 \pm 2.36 \pm 1.44$ | 1.6 | [51] |
| Dileptons | Run I | CDF | 0.1 | 8 | 16 | $167.4 \pm 10.3 \pm 4.9$ | 6.8 | [52] |
| Dileptons | Run I | D0 | 0.1 | 6 | 25 | $168.4 \pm 12.3 \pm 3.6$ | 7.6 | [53] |
| $\mathbb{E}_{T}+$ jets | Run II | CDF | 5.7 | 1432 | 32 | $172.32 \pm 1.80 \pm 1.82$ | 1.5 | [54] |
| Decay length | Run II | CDF | 1.9 | 375 | 30 | $166.90 \pm 9.00 \pm 2.82$ | 5.7 | [55] |
| Combination |  |  | $\leq 5.8$ | 7420 | 44 | $173.18 \pm 0.56 \pm 0.75$ | 0.54 |  |

maximizes the improvement in the combination, and because enough information is available to separate the components of systematic uncertainty for proper treatment in the combination.

The D0 measurement from 2005 in the alljets channel (Run I) [56] of $m_{t}=178.5 \pm 13.7$ (stat) $\pm 7.7$ (syst) GeV (total uncertainty of $8.8 \%$ ) is not included in the combination because some subcomponents of the systematic uncertainty are not available.

The CDF measurement from Run II based on decaylength analysis [55] differs from the others in that it uses the mean decay length of $B$ hadrons in $b$-tagged lepton + jets events as the $m_{t}$-sensitive variable. It is independent of energy information in the calorimeter, and its main source of systematic uncertainty is uncorrelated with the dominant ones from the jet energy scale calibration in other measurements. This measurement of $m_{t}$ is essentially uncorrelated with the higher precision CDF result from the lepton + jets channel. The overlap between the data samples used for the decay-length method and the lepton + jets sample has therefore no effect.

## B. Data

The data were collected with the CDF [57] and D0 [58,59] detectors at the Tevatron $p \bar{p}$ collider at Fermilab between 1992 and 2009. The Tevatron "center-of-mass" energy was 1.8 TeV in Run I from 1992 to 1996 and 1.96 TeV in Run II from 2001. A silicon microstrip tracker around the beam pipe at the center of each detector was used to reconstruct charged-particle tracks (only in Run II at D0). Tracks spatially matched to calorimeter jets are checked for originating from a secondary vertex, or for evidence that they originate from decays of long-lived heavy-flavor hadrons containing $b$ quarks from the decay of top quarks $[57,60]$. Electrons and jets produce particle
showers in the calorimeters, and the collected information is used to measure their energies. Muons traverse the calorimeters and outer muon detectors that are used to reconstruct their tracks. Both CDF and D0 have central axial magnetic fields in the tracking region (D0 only in Run II), in which the momenta of charged particles are determined from the curvature of their tracks. The CDF magnet has a diameter of 3 m and extends 4.8 m along the beam line, with a field strength of 1.4 T , and the D0 magnet has a diameter of 1.0 m and length of 2.7 m to fit inside the Run I calorimeter with a field strength of 2.0 T . The CDF detector's larger tracking volume with a higher density of measurements gives better transverse-momentum resolution for charged-particle tracks. The transverse-momentum resolution is $\approx 3.5 \%$ at CDF and $\approx 10 \%$ at D 0 for a muon with $p_{T}=50 \mathrm{GeV}$. The trigger and event-selection criteria depend on the $t \bar{t}$ final states, details of which appear in the publications listed in Table I. The experiments collected $\mathcal{O}\left(10^{14}\right)$ hard collisions, from which 7420 events are selected because they have the characteristics expected for $t \bar{t}$ pairs, of which $\approx 56 \%$ are expected to be true $t \bar{t}$ events.

## C. Models for $\boldsymbol{t} \overline{\boldsymbol{t}}$ signal

The $t \bar{t}$ signal in Run I was simulated using the LO generator HERWIG [61] with the $\mathrm{MRSD}_{0}^{\prime}$ [62] and CTEQ4M [63] parton distribution functions (PDF) used by CDF and D0, respectively. The HERWIG generator implements the hard-scattering processes $q \bar{q} \rightarrow t \bar{t}$ and $g g \rightarrow t \bar{t}$, adding initial-state and final-state radiation through leading-log QCD evolution [64]. The top quark and $W$ boson in HERWIG decay according to the branching fractions listed by the Particle Data Group [7], and the final-state partons are subsequently fragmented into jets. The MC events are then processed through a fast
simulation or a GEANT model [65] of the detectors and then through event reconstruction programs.

For the $t \bar{t}$ signal in Run II, CDF uses PYthia [66] with the CTEQ5L [67] PDF, and D0 uses the leading-log generator AlPGEN [68] with the CTEQ6L1 [69] PDF and PYTHIA for parton showering. ALPGEN contains more tree-level graphs in higher-order $\alpha_{s}$ than PYTHIA. ALPGEN has parton-jet matching [70], which avoids double counting of partons in overlapping regions of jet kinematics. CDF sets the event generation factorization and renormalization scales $Q^{2}$ to $m_{t}^{2}+p_{\perp}^{2}+\left(P_{1}^{2}+P_{2}^{2}\right) / 2$, where $p_{\perp}$ is the transverse momentum characterizing the scattering process, and $P_{1}^{2}$ and $P_{2}^{2}$ are the virtualities of the incoming partons. D0 sets the scales to $m_{t}^{2}+\left\langle p_{T}^{2}\right\rangle$, where $\left\langle p_{T}^{2}\right\rangle$ is the average of the square of transverse momentum of all other light partons produced in association with the $t \bar{t}$ pair. The PYTHIA model treats each step of the $t \bar{t}$ decay chain ( $t \rightarrow W b, W \rightarrow \ell \nu$ or $q \bar{q}^{\prime}$ ) separately and does not preserve spin correlations. ALPGEN uses exact matrix elements for each step and thereby correctly describes the spin information of the final-state partons. The fragments of the proton and antiproton or "underlying event" are added separately to each hard collision. CDF uses the "Tune A" settings [71] in PYTHIA while D0 uses a modified version of the tune. Both collaborations use angular ordering for modeling parton showering in PYTHIA, and not $p_{T}$-ordered models. The underlying event is therefore not interleaved with the parton showers as in models of color reconnection [72].

## D. Background models

In the lepton + jets channel, the dominant background is from $W+$ jets production. Smaller contributions arise from multijet events, $Z+$ jets, single top-quark ( $t q b$ and $t b$ ), and diboson production ( $W W, W Z$, and $Z Z$ ). The alljets channel has mainly multijet events as background. The largest background in the dilepton channel is from $Z+$ jets events, which include Drell-Yan production. Backgrounds from diboson production and from events with jets identified as leptons are very small in the dilepton channel. The $\mathscr{E}_{T}+$ jets channel has multijet events and $W+$ jets as main backgrounds.

In all channels contributions from multijet events are modeled using data. Most other background sources are modeled through MC simulation. In Run I, both collaborations used vecbos [73] to model $W+$ jets events. VECBOS is a precursor of ALPGEN and provides one of the first models of events with many high-momentum final-state partons. PYTHIA was used to model $Z+$ jets, Drell-Yan, and diboson processes. Background from events with a single top quark was negligible. In Run II, both collaborations used ALPGEN for the simulation of the $W+$ jets background. The treatment of heavy-flavor jets is implemented more accurately in ALPGEN, and parton-jet matching also improves the simulation. For the $Z+$ jets
background, CDF uses PYTHIA and D0 uses alpgen. For dibosons, both collaborations use PYTHIA. Processes with a single top quark are modeled by CDF using MADEVENT [74] (based on MADGRAPH [75]) and by D0 with SINGLETOP [76] (based on COMPHEP [77]).

The uncertainty in the description of the $W+$ jets background has three main components: (i) the uncertainty on the scale $Q^{2}$, which affects both the overall normalization and the differential jet distributions in pseudorapidity $\eta$ [78] and $p_{T}$; (ii) the uncertainty in the correction for flavor content of jets to higher order; and (iii) the limitation in the MC model we are using to reproduce the jet $p_{T}$ and $\eta$ distributions in data at low $p_{T}$ and large $|\eta|$.

## E. Jet properties

After the top quarks decay, the final-state quarks and gluons hadronize to produce multiple charged and neutral particles that traverse the central tracking systems into the calorimeters, where they produce many lower-momentum particles through interactions in the absorbers of the calorimeters. The observed particles tend to cluster in jets that can be assigned to the initial partons. For jet reconstruction, the CDF Collaboration uses a clustering algorithm in ( $\eta, \phi$ ) space [79] with a cone radius of

$$
\mathrm{CDF} \quad \mathcal{R}=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}=0.4,
$$

where $\phi$ is the azimuthal angle around the beam line, $\eta$ is the pseudorapidity, and $\Delta \eta$ or $\Delta \phi$ are the widths of the cone. D0 uses a midpoint iterative seed-based cone algorithm in ( $y, \phi$ ) space [80] with a radius defined by

$$
\text { D } 0 \quad \mathcal{R}=\sqrt{(\Delta y)^{2}+(\Delta \phi)^{2}}=0.5,
$$

where the rapidity $y=1 / 2 \ln \left(\left(E+p_{L}\right) /\left(E-p_{L}\right)\right), E$ is the jet energy, and $p_{L}$ is its longitudinal momentum component.

The jet energy resolution in the central region $(|\eta|<1)$ is approximately the same for CDF and D0; for CDF it is $\sigma\left(E_{T}\right) / E_{T}=50 \% / \sqrt{E_{T}(\mathrm{GeV})} \oplus 3 \%$. For jets in the forward region, however, the energy resolution at D0 is similar to that in the central region, while at CDF it is not as $\operatorname{good}\left[\sigma\left(E_{T}\right) / E_{T}=70 \% / \sqrt{E_{T}(\mathrm{GeV})} \oplus 4 \%\right]$. CDF's calorimeter covers $|\eta|<3.8$, whereas D0's calorimeter covers $|\eta|<4.2$. The D0 calorimeter is more homogeneous, so that the imbalance in transverse momentum (see Sec. II G) usually has better resolution at D0. For both CDF and D0, to reject jets with mismeasured energy, selections on energy deposition are required when clustering the energy from the calorimeter cells into jets. When a muon is reconstructed within the jet cone, a correction is applied to the jet energy to account for the muon and its associated neutrino assumed to arise from heavy-quark decay.

Jet energy scale calibrations are applied after jet reconstruction. CDF calibrates the transverse momentum using
test-beam data and single-particle simulated events and corrects the jet energy to the parton level. Consequently, CDF does not calibrate the jet energy scale in MC events. D0 calibrates the energy using photon + jets and two-jet data and calibrates jets in data as well as in MC to the observed particle level. Particle jets are clustered from stable particles after fragmentation, including particles from the underlying event, but excluding undetected energy from muons and neutrinos.

CDF's jet calibration [81] applies two scale factors and three offsets to convert the measured transverse momentum of a jet to that of the parton that initiated the jet. D0's jet calibration [82] applies three scale factors and one offset to the jet energy to convert to the particle jet energy scale. The calibrations are expressed as follows:

$$
\begin{aligned}
& \mathrm{CDF} p_{T}^{\mathrm{parton}} \\
&=\frac{p_{T}^{\mathrm{jet}} R_{\mathrm{rel}}-C_{\mathrm{MI}}}{R_{\mathrm{abs}}}-C_{\mathrm{UE}}+C_{\mathrm{OC}} \\
& \mathrm{D} 0 E^{\mathrm{particle}}
\end{aligned}=\frac{E^{\mathrm{jet}}-C_{\mathrm{MI}, \mathrm{UE}}}{R_{\mathrm{abs}} R_{\mathrm{rel}} F_{\mathrm{OC}}} .
$$

The absolute response $R_{\mathrm{abs}}$ corrects for energy lost in uninstrumented regions between calorimeter modules, for differences between electromagnetically and hadronically interacting particles, as well as for module-to-module irregularities. The relative response $R_{\text {rel }}$ is a scale factor that corrects forward relative to central jets and $C_{\mathrm{MI}}$ is a correction for multiple interactions in the same bunch crossing. The function $C_{\mathrm{UE}}$ is a correction for the jet energy added from the underlying event. D0 has one offset correction, $C_{\mathrm{MI}, \mathrm{UE}}$, which includes the effects of multiple interactions, the underlying event, noise from radioactive decays of the uranium absorber, and the effect of collisions from previous bunch crossings (pileup). The functions $C_{\mathrm{OC}}$ and $F_{\mathrm{OC}}$ are corrections for shower particles scattered in or out of the cone of radius $\mathcal{R}$. CDF's correction accounts for MC modeling that affects how the parton energy is translated into particle jet energy, whereas D0's correction accounts for a detector effect caused by the finite cell size in the calorimeter coupled with the cone size for the jet algorithm. The combined jet energy scale corrections increase the measured jet energies by about $20 \%-50 \%$, depending on $p_{T}$ and $\eta$.

The overall uncertainties on the jet energy scale corrections vary from about $2.7 \%$ for CDF and $1.1 \%$ for D0 for central jets of transverse energy of 100 GeV to $3.3 \%$ for CDF and $2.2 \%$ for D0 for forward jets. Central jets of 25 GeV have correction uncertainties of $5.9 \%$ for CDF and $1.4 \%$ for D0. For both experiments, the uncertainty on the corrections for absolute response $R_{\text {abs }}$ dominate these uncertainties.

At D0, the jet energy resolution in data is lower than predicted by the detector simulation. Therefore, the energies of MC jets are smeared so that the resulting resolution in MC matches that in data. Similarly, the reconstruction efficiency for jets in data is lower than is predicted by the
detector simulation, so an appropriate fraction of MC jets are randomly removed. Both effects are corrected for as functions of jet $p_{T}$ and pseudorapidity.

D0 Run II analyses include an energy correction to simulated jets that depends on jet flavor. There are corrections for $b$ jets, other-quark flavor jets ( $u, d, s$, and $c$ ), and gluon jets implemented in both the lepton + jets and dilepton analyses. Such corrections refine the simulation by improving the matching of jet energies in MC to data. The differences arise from the varying electromagnetic fractions and widths of the jets. The corrections depend on jet transverse energy and pseudorapidity and range from $-6 \%$ to $+2 \%$ [25].

Both collaborations perform an in situ jet energy scale calibration in lepton + jets events for the matrix-element mass extraction of $m_{t}$, and in CDF's alljets and $\mathscr{E}_{T}+$ jets measurements of $m_{t}$. The invariant mass of the two jets is constrained to a Breit-Wigner distribution for the $W \rightarrow q \bar{q}^{\prime}$ decay, set to the world average value for the $W$-boson mass [7]. The energies of all jets in the event are then rescaled to complete this calibration.

## F. $\boldsymbol{b}$-quark jet properties

To separate top-quark events from background and to decrease the ambiguity in jet-to-parton matching, it is important to identify $b$-quark jets. Every $t \bar{t}$ event has two $b$ jets, whereas such jets are rare in background. As $B$ hadrons have a mean lifetime of $\approx 10^{-12} \mathrm{~s}, b$ jets can be tagged through secondary vertices of the $B$ decay a few mm away from the primary $p \bar{p}$ interaction. CDF's $b$-tagging algorithm uses the significance of the displacement of the secondary vertex in the transverse $(r, \phi)$ plane for the lepton + jets and $\mathscr{E}_{T}+$ jets channels [57], as well as a jet-probability algorithm for $\mathscr{E}_{T}+$ jets events [83]. One parameter defines the significance of the separation of the primary and secondary vertices for events with one and two $b$ jets. For jets that are within the acceptance of the silicon microstrip tracker (i.e., "taggable" jets), this algorithm identifies $50 \%$ of real $b$ jets and $9 \%$ of real charm jets, while falsely tagging $1 \%$ of light jets. D0 tags jets by combining nine track and secondary-vertex-related variables using a neural network [60]. For jets within the acceptance of the silicon microstrip detector, this yields efficiencies of $65 \%$ and $20 \%$ for real $b$ and charm jets, respectively, while falsely tagging $3 \%$ of light jets.

To identify heavy-flavor jets in data and in MC events, the tagging algorithm is applied by CDF and D0 directly to the jets, except for simulated $W+$ light jets events, where CDF uses tag-rate functions measured in multijet data, since the rate for directly tagged MC events is very low. After applying direct tagging to $b$ and $c$ jets in MC events, D0 corrects the tagging efficiencies to match those observed in data by randomly dropping the tagging of $13 \%$ of such jets. For light-flavor jets, D0 assigns a per jet mistag weight.

## G. Properties of other event observables

The uncertainty on $m_{t}$ depends not only on an accurate measurement of jet energies and proper assignment of flavor but also on the reconstruction and calibration of the other elements of the event, including electrons, muons, and the imbalance in transverse momentum, taking into account the presence of any simultaneous $p \bar{p}$ interactions in the same bunch crossing.

The mean number of $p \bar{p}$ collisions per bunch crossing is $\approx 2$ in Run I and $\approx 5$ in Run II. Such additional collisions affect the observed characteristics of the hard scatter of interest and must be included in the MC simulation. These extra collisions result mostly in the production of low- $p_{T}$ particles. CDF simulates such additional interactions using the PYTHIA model of minimum-bias events and overlays them onto the hard scatters using a Poisson mean appropriate to the instantaneous luminosity of the data. In a similar manner D0 overlays randomly triggered data events with the same luminosity profile as the data onto the MC simulated events.

Electrons are identified by matching clusters of energy deposited in the electromagnetic layers of the calorimeters with tracks that point from the primary collision vertex to the clusters. The spatial shapes of the showers must agree with those expected for electrons, as studied in test-beam data. The energy of an electron is determined as a combination of the total energy of the cluster and the momentum measured from the curvature of the matching track. The reconstruction efficiency is determined using $Z \rightarrow e e$ data by identifying one tight charged lepton as a tag and using the other charged lepton as a probe (tag-and-probe method). The electron energy is also recalibrated using such $Z$ events.

Muons are reconstructed from a central track and matched to a track in the outer muon chambers. In D0, both the inner and outer trajectories pass through magnetic fields, and so the transverse momenta of the two are therefore required to match. The reconstruction efficiency and calibration of $p_{T}$ are determined using a tag-and-probe method applied on $J / \psi \rightarrow \mu \mu$ and $Z \rightarrow \mu \mu$ events in a manner similar to that used for electrons.

As indicated above, all $t \bar{t}$ decay channels except for alljets events have a large $\mathscr{E}_{T}$. All jet energy calibration corrections are also propagated to $\mathscr{E}_{T}$ in each event.

## III. COMBINATION OF MASS MEASUREMENTS

## A. BLUE combination method

The basic idea of the technique, called the best linear unbiased estimator (BLUE) method [32-34], used to obtain the combined mass $m_{t}^{\text {comb }}$, an "estimator" of the true mass $m_{t}^{\text {true }}$, is to calculate a linear weighted sum of the results from separate measurements:

$$
\begin{equation*}
m_{t}^{\mathrm{comb}}=\sum_{i=1}^{12} w_{i} m_{t}^{i} \tag{1}
\end{equation*}
$$

The $m_{t}^{i}$ are the 12 CDF and D 0 measurements $i$ of $m_{t}$ and

$$
\begin{equation*}
\sum_{i=1}^{12} w_{i}=1 \tag{2}
\end{equation*}
$$

The weights are determined using the value of $m_{t}^{\text {comb }}$ that minimizes the squared difference relative to the unknown true value $m_{t}^{\text {true }}$ :

$$
\begin{equation*}
\left(m_{t}^{\mathrm{comb}}-m_{t}^{\mathrm{true}}\right)^{2}=\operatorname{Variance}\left(m_{t}^{\mathrm{comb}}\right)+\left[\operatorname{Bias}\left(m_{t}^{\mathrm{comb}}\right)\right]^{2} \tag{3}
\end{equation*}
$$

where the two terms represent the weighted variance and bias in the 12 input $m_{t}$ values with

$$
\begin{equation*}
\operatorname{Variance}\left(m_{t}^{\mathrm{comb}}\right)=\sum_{i=1}^{12} w_{i}^{2} \operatorname{Variance}\left(m_{t}^{i}\right) \tag{4}
\end{equation*}
$$

and

$$
\begin{equation*}
\operatorname{Variance}\left(m_{t}^{i}\right)=\left[\sigma\left(m_{t}^{i}\right)\right]^{2} \tag{5}
\end{equation*}
$$

where $\sigma\left(m_{t}^{i}\right)$ are the uncertainties on the 12 input values given in Table I.

On average, we expect the input mass measurements to be unbiased, and we therefore assume

$$
\begin{equation*}
\operatorname{Bias}\left(m_{t}^{\mathrm{comb}}\right)=\sum_{i=1}^{12} w_{i} \operatorname{Bias}\left(m_{t}^{i}\right)=0 \tag{6}
\end{equation*}
$$

Equation (3) shows that the BLUE method defines the best estimate through a minimization of the variance of $m_{t}$ for an assumed unbiased set of measurements. The minimum corresponds to setting the weights to

$$
\begin{equation*}
w_{i}=\frac{1 / \operatorname{Variance}\left(m_{t}^{i}\right)}{\sum_{i=1}^{12} 1 / \operatorname{Variance}\left(m_{t}^{i}\right)} \tag{7}
\end{equation*}
$$

for uncorrelated input values. Since the input $m_{t}$ values are correlated, the variance in Eq. (4) has to be replaced with a covariance matrix:
$\operatorname{Variance}\left(m_{t}^{\mathrm{comb}}\right)=\sum_{i=1}^{12} \sum_{j=1}^{12} w_{i} w_{j} \operatorname{Covariance}\left(m_{t}^{i}, m_{t}^{j}\right)$,
which is defined as

$$
\begin{equation*}
\operatorname{Covariance}\left(m_{t}^{i}, m_{t}^{j}\right)=\left[\sigma\left(m_{t}^{i} m_{t}^{j}\right)\right]^{2}-\sigma\left(m_{t}^{i}\right) \sigma\left(m_{t}^{j}\right) \tag{9}
\end{equation*}
$$

Minimizing Eq. (3) yields

$$
\begin{equation*}
w_{i}=\frac{\sum_{j=1}^{12} \text { Covariance }^{-1}\left(m_{t}^{i}, m_{t}^{j}\right)}{\sum_{i=1}^{12} \sum_{j=1}^{12} \text { Covariance }^{-1}\left(m_{t}^{i}, m_{t}^{j}\right)}, \tag{10}
\end{equation*}
$$

where Covariance ${ }^{-1}\left(m_{t}^{i}, m_{t}^{j}\right)$ are the elements of the inverse of the covariance matrix (also known as the error matrix), and

Covariance $\left(m_{t}^{i}, m_{t}^{j}\right)=$ Correlation $\left(m_{t}^{i}, m_{t}^{j}\right) \sigma\left(m_{t}^{i}\right) \sigma\left(m_{t}^{j}\right)$
with Correlation $\left(m_{t}^{i}, m_{t}^{j}\right)$ the correlation coefficient between $m_{t}^{i}$ and $m_{t}^{j}$. The following sections show how the

TABLE II. The uncertainty in GeV from each component for the 12 measurements of $m_{t}$ and the resulting Tevatron combination. The total uncertainties are obtained by adding the components in quadrature. The entries " $\mathrm{n} / \mathrm{a}$ " stand for "not applicable" and " $\mathrm{n} / \mathrm{e}$ " for "not evaluated." The nonevaluated uncertainties were not considered as significant sources of uncertainty for Run I measurements.

|  |  |  |  | Light-jet response (2) | $\begin{aligned} & . \tilde{0} \\ & .0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 1 \\ & 0 \\ & 0 \\ & 0.1 \end{aligned}$ | $\begin{aligned} & \stackrel{\rightharpoonup}{0} \\ & \stackrel{4}{0} \end{aligned}$ | $\begin{aligned} & \stackrel{0}{0} \\ & \stackrel{0}{2} \\ & \stackrel{0}{0} \\ & \frac{0}{0} \\ & \frac{0}{2} \end{aligned}$ | $\begin{aligned} & \stackrel{n}{0} \\ & \stackrel{0}{\infty} \\ & \stackrel{0}{3} \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 . \\ & 0 \\ & 0 \end{aligned}$ | In situ light-jet calibration |  |  |  | Multiple interactions model |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Channel | Run | Expt. |  |  | nergy | ale | ste |  |  |  |  | Othe | yst | atics |  |  |  |  |  |  |
| Lepton + jets | II | CDF | 0.41 | 0.01 | 0.27 | n/a | 0.23 | 0.13 | 0.58 | 0.00 | 0.14 | 0.56 | 0.10 | 0.27 | 0.06 | 0.10 | 0.65 | 0.80 | 0.67 | 1.23 |
| Lepton + jets | II | D0 | n/a | 0.63 | n/a | n/a | 0.07 | 0.26 | 0.46 | 0.36 | 0.18 | 0.77 | 0.05 | 0.19 | 0.23 | 0.16 | 0.83 | 0.83 | 0.94 | 1.50 |
| Lepton + jets | I | CDF | 3.4 | 0.7 | 2.7 | n/a | 0.6 | n/e | $\mathrm{n} / \mathrm{a}$ | n/e | n/e | 2.7 | n/e | 1.3 | n/e | 0.0 | 5.1 | 4.4 | 2.8 | 7.3 |
| Lepton + jets | I | D0 | n/a | 2.5 | 2.0 | 1.3 | 0.7 | n/e | n/a | n/e | n/e | 1.3 | n/e | 1.0 | n/e | 0.6 | 3.6 | 3.5 | 1.6 | 5.3 |
| Alljets | II | CDF | 0.38 | 0.04 | 0.24 | n/a | 0.15 | 0.03 | 0.95 | 0.00 | n/a | 0.64 | 0.08 | 0.00 | 0.56 | 0.38 | 1.43 | 1.06 | 0.91 | 2.00 |
| Alljets | I | CDF | 4.0 | 0.3 | 3.0 | $\mathrm{n} / \mathrm{a}$ | 0.6 | n/e | $\mathrm{n} / \mathrm{a}$ | n/e | n/a | 2.1 | n/e | 1.7 | n/e | 0.6 | 10.0 | 5.0 | 2.6 | 11.5 |
| Dileptons | II | CDF | 2.01 | 0.58 | 2.13 | n/a | 0.33 | 0.14 | n/a | 0.00 | 0.27 | 0.80 | 0.23 | 0.24 | 0.14 | 0.12 | 1.95 | 3.01 | 0.88 | 3.69 |
| Dileptons | II | D0 | n/a | 0.56 | n/a | n/a | 0.20 | 0.40 | 0.55 | 0.50 | 0.35 | 0.86 | 0.00 | 0.00 | 0.20 | 0.51 | 2.36 | 0.90 | 1.11 | 2.76 |
| Dileptons | I | CDF | 2.7 | 0.6 | 2.6 | n/a | 0.8 | n/e | n/a | n/e | n/e | 3.0 | n/e | 0.3 | n/e | 0.7 | 10.3 | 3.9 | 3.0 | 11.4 |
| Dileptons | I | D0 | n/a | 1.1 | 2.0 | 1.3 | 0.7 | n/e | n/a | n/e | n/e | 1.9 | n/e | 1.1 | n/e | 1.1 | 12.3 | 2.7 | 2.3 | 12.8 |
| $\mathscr{L S}_{T}+$ jets | II | CDF | 0.45 | 0.05 | 0.20 | n/a | 0.00 | 0.12 | 1.54 | 0.00 | n/a | 0.78 | 0.16 | 0.00 | 0.12 | 0.14 | 1.80 | 1.64 | 0.78 | 2.56 |
| Decay length | II | CDF | 0.24 | 0.06 | n/a | n/a | 0.15 | n/e | n/a | 0.00 | n/a | 0.90 | 0.00 | 0.80 | 0.20 | 2.50 | 9.00 | 0.25 | 2.80 | 9.43 |
| Tevatron combination |  |  | 0.12 | 0.19 | 0.04 | 0.00 | 0.15 | 0.12 | 0.39 | 0.11 | 0.10 | 0.51 | 0.00 | 0.14 | 0.11 | 0.09 | 0.56 | 0.49 | 0.57 | 0.94 |

correlation matrix is derived by examining the uncertainty components and their individual correlations.

## B. Measurement uncertainties

The uncertainty on any $m_{t}$ measurement has a statistical component from the limited number of events available for the measurement and a systematic component from the uncertainties assigned to the calibration of input quantities, to the model of the signal, and to the calibration of the mass extraction method. Since the first measurements of $m_{t}$ [4,5], the systematic component has been slightly larger than the statistical one. As more data became available, the statistical uncertainties on $m_{t}$ improved as did the calibrations of systematic uncertainty, and the two components therefore improved together.

The systematic uncertainty on each $m_{t}$ measurement in this combination is divided into 14 parts. Some of them have origin in only one source, whereas others include several related sources of uncertainties. For the latter the patterns of correlation among different channels, Tevatron Run I and Run II, or experiments are the same for all sources included in these systematic components. The uncertainty on jet energy scale (JES), on the other hand, is split into seven components, which do not apply to all measurements, given the significantly different approaches to jet energy calibration between CDF and D0 and the change in the D0 procedure between Run I and Run II.

Table II gives the uncertainty of each of the 12 top-quark mass measurements for the different contributions to uncertainty and their effect on the final combination. The components of uncertainty are defined in the following and can be classified as uncertainties in detector response (jet energy scale, jet and lepton modeling), uncertainties from modeling signal and background (signal modeling, multiple interactions model, background estimated from theory, and background based on data), uncertainties from method of mass extraction, and statistical uncertainties. A detailed description of the methods to evaluate these systematic uncertainties is presented in the Appendix.

## 1. Jet energy scale

## a. Light-jet response (1)

One subcomponent of the uncertainty in JES covers the absolute calibration for CDF's Run I and Run II measurements. It also includes small contributions from the uncertainties associated with modeling multiple interactions within a single bunch crossing and corrections for the underlying event.

## b. Light-jet response (2)

Another subcomponent of this uncertainty includes D0's Run I and Run II calibrations of absolute response (energy dependent), the relative response ( $\eta$ dependent), and the
out-of-cone showering correction that is a detector effect. This uncertainty term for CDF includes only the small relative response calibration ( $\eta$ dependent) for Run I and Run II.

## c. Out-of-cone correction

This subcomponent of the JES uncertainty quantifies the out-of-cone showering corrections to the MC showers for all of CDF's and for D0's Run I measurements that are obtained by varying the model for light-quark fragmentation.

## d. Offset

This subcomponent originates from the offset in D0's Run I calibration, which corrects for noise from uranium decay, pileup from previous collisions, and for multiple interactions and the model for the underlying event. In Run I, the uncertainties are large, but in Run II, owing to the smaller integration time for calorimeter electronics, they are negligible. CDF's calorimeter does not have the same sources of noise and sensitivity to pileup as D0, so CDF measurements do not have this term.

## e. Model for $b$ jets

This subcomponent comes from the uncertainty on the semileptonic branching fraction in $b$ decays and from differences between two models of $b$-jet hadronization.

## f. Response to $b / q / g$ jets

This subcomponent accounts for the difference in the electromagnetic versus hadronic response of $b$ jets, lightquark jets, and gluon jets. CDF corrects for jet flavor as part of the main calibration, and defines the uncertainty based on the remaining difference in response between $b$ jets and light-flavor jets, whereas D0 corrects the response for $b$, light-quark $(u, d, s$, and $c)$, and gluon jets as a function of jet $p_{T}$ and $\eta$.

## g. In situ light-jet calibration

The last part of the uncertainty in the jet energy scale is from the in situ calibration of $m_{t}$. It corresponds to the statistical uncertainty from the limited number of events used in the fit when using the $W$-boson mass to constrain the energies of the light quarks from the $W$ decay.

## 2. Jet modeling

The uncertainty in jet modeling has two components for D0. This uncertainty is negligible for CDF.
(i) The jet energy resolution is smeared for MC jets to match the resolution observed in data, and the uncertainty on the smearing functions is propagated to $m_{t}$.
(ii) The identification efficiency in MC events is corrected to match that found in data, and the uncertainty on the correction functions is propagated to $m_{t}$.

## 3. Lepton modeling

This uncertainty has two components:
(i) The electron and muon $p_{T}$ scales are calibrated to the $J / \psi$ and $Z$-boson mass by both CDF and D0. This uncertainty on the calibration is included in the measurements of $m_{t}$.
(ii) D0 smears the muon momentum resolution in MC events to match that in data, and the uncertainty on this correction is included in this term. The uncertainty on the electron resolution has a negligible impact on the measurements of $m_{t}$.

## 4. Signal modeling

There are six components to this uncertainty. They are combined into one term because the correlations between channels are similar for each component:
(i) Knowledge of the PDF parametrization.
(ii) The quark annihilation and gluon fusion fractions that differ significantly between leading-log and next-to-leading-order (NLO) QCD calculations (Run II).
(iii) The amount of initial- and final-state radiation in MC signal events differs from that in data and is adjusted through the value of $\Lambda_{\mathrm{QCD}}$ used in the shower and the scales of time and spacelike showers.
(iv) Higher-order QCD corrections to initial- and finalstate radiation differ from precise parton-level models, and this is not accounted for by the choice of scale for the calculations (Run II).
(v) Our model for jet hadronization is based on angular ordering in PYTHIA with Tune A underlyingevent tuning. Parton showering and the underlying event can also be simulated with HERWIG and JIMMY $[84,85]$. The effect of the difference on $m_{t}$ between the two models is included in this term.
(vi) Final-state partons and remnants of the protons and antiprotons are connected through color strings, which affect the distributions of jets. Since this effect is not included in the model for the $t \bar{t}$ signal, the value of $m_{t}$ has an uncertainty from this omission (Run II).

## 5. Multiple interactions model

The number of soft $p \bar{p}$ events overlaid on each MC event has a Poisson distribution. The mean number does not equal exactly the number seen in data since the luminosity increased as the Tevatron run progressed. The top-quark mass is measured as a function of the number of multiple interactions in signal events by CDF, the signal MC events are reweighted to match the distribution seen in data by D0, and the related uncertainties are included here.

## 6. Background from theory

There are four components in this uncertainty:
(i) Difference between NLO calculations of the fraction of heavy-flavor jets in $W+$ jets events. The ALPGEN model underestimates this fraction.
(ii) Impact of factorization and renormalization scales on the $W+$ jets simulation, which affects the background model for distributions characterizing jets.
(iii) The theoretical cross sections used to normalize all MC estimated background processes (except for $W+$ jets for CDF and D0 lepton + jets measurements, and Drell-Yan production for CDF dilepton measurements).
(iv) Impact of difference between the MC modeling of background kinematic distributions and those observed in data.

## 7. Background based on data

This refers primarily to uncertainties from the normalization of certain background components to data. These include multijet backgrounds in the lepton + jets, alljets, and $\mathscr{E}_{T}+$ jets analyses, the $W+$ jets background in the D0 lepton + jets analyses, and the Drell-Yan backgrounds in the CDF dilepton analyses.

D0 also considers the following four components of uncertainty:
(i) The uncertainty from correcting the MC events to match the trigger efficiency in data, which is based on the turn-on response for each trigger element.
(ii) The uncertainty from applying tag-rate and taggability corrections to MC events to make the efficiencies match the data for each jet flavor.
(iii) The uncertainty on the fraction of multijet events included in the pseudoexperiments used for calibration.

## 8. Calibration method

The extracted values of $m_{t}$ are calibrated using a straight-line fit to the relationship between input mass and measured mass in simulated pseudoexperiments. This term includes the systematic uncertainties from the slope and offset of this calibration.

## 9. Statistical uncertainty

The statistical uncertainties are determined from the number of data events in each of the 12 measurements.

Figure 5 shows the relative contribution for each major uncertainty to the analysis channels in Run II. The Appendix provides more detail on how each of the sources of the uncertainties is estimated.

## C. Uncertainty correlations

Tables III and IV indicate how uncertainties are correlated between measurements. There are seven patterns of correlation:


FIG. 5 (color online). The average uncertainties for CDF and D0 for each Run II measurement and for the Tevatron combination, separated according to major components. (See Table VIII in the Appendix for details on the systematic categories. In this figure, the jet and lepton modeling systematic uncertainties are grouped into the modeling background category.)
(i) Statistical uncertainty and calibration method uncertainty are not correlated among the measurements.
(ii) Correlations among D0 measurements that implement the same final jet energy corrections for the uncertainty from in situ light-jet calibration.
(iii) Correlations among CDF measurements that use the same data samples for the uncertainty from background based on data.
(iv) Correlations among all measurements in the same $t \bar{t}$ decay channel for the uncertainty from background estimated from theory.
(v) Correlations of measurements within the same experiment for a given run period for the uncertainties from light-jet response (2), offset, response to $b / q / g$ jets, jet modeling, lepton modeling, and multiple interactions model.
(vi) Correlations for measurements within the same experiment such as the uncertainty from light-jet response (1).
(vii) Correlations among all measurements such as the uncertainties from out-of-cone correction, model for $b$ jets, and signal modeling.
We assume that all sources correspond to either no or $100 \%$ correlation. A check of this assumption (see Sec. IV B) shows that it has a negligible effect on the combined value and uncertainty of $m_{t}$.

## D. Measurement correlations

The uncertainties shown in Table II and their correlations shown in Tables III and IV provide the correlations among the 12 input values of $m_{t}$. The correlation matrix for these measurements, as returned by the combination procedure, is shown in Table V. The inversion of the covariance matrix built with the correlation matrix defines the measurement weights, as described in Sec. III A.

TABLE III. Correlations in systematic uncertainties (in percent) among the different measurements of $m_{t}$.
(20

Not correlated among any measurements
In situ light-jet calibration (JES)

| Lepton + jets | Run II | CDF | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Lepton + jets | Run II | D0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 |
| Lepton + jets | Run I | CDF | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Lepton + jets | Run I | D0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Alljets | Run II | CDF | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Alljets | Run I | CDF | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dileptons | Run II | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 |
| Dileptons | Run II | D0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 |
| Dileptons | Run I | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 |
| Dileptons | Run I | D0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 |
| $\mathbb{E}_{T}+$ jets | Run II | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 |
| Decay length | Run II | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| Background based on data |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Lepton + jets | Run II | CDF | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| Lepton + jets | Run II | D0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Lepton + jets | Run I | CDF | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Lepton + jets | Run I | D0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Alljets | Run II | CDF | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Alljets | Run I | CDF | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dileptons | Run II | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 |
| Dileptons | Run II | D0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 |
| Dileptons | Run I | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 |
| Dileptons | Run I | D0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 |
| $\mathbb{E}_{T}+$ jets | Run II | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 |
| Decay length | Run II | CDF | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| Background from theory |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| Lepton + jets | Run II | CDF | 100 | 100 | 100 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| Lepton + jets | Run II | D0 | 100 | 100 | 100 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| Lepton + jets | Run I | CDF | 100 | 100 | 100 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| Lepton + jets | Run I | D0 | 100 | 100 | 100 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |
| Alljets | Run II | CDF | 0 | 0 | 0 | 0 | 100 | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| Alljets | Run I | CDF | 0 | 0 | 0 | 0 | 100 | 100 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dileptons | Run II | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 100 | 100 | 0 | 0 |
| Dileptons | Run II | D0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 100 | 100 | 0 | 0 |
| Dileptons | Run I | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 100 | 100 | 0 | 0 |
| Dileptons | Run I | D0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 100 | 100 | 100 | 0 | 0 |
| $\mathbb{E}_{T}+$ jets | Run II | CDF | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 | 0 |
| Decay length | Run II | CDF | 100 | 100 | 100 | 100 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 100 |


|  |  |  |  | ht-j | respo |  |  | Offs |  |  | pon | $b /$ | jets |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  |  | mode |  | Lept | deling |  | ultipl | era | m |  |  |
| Lepton + jets | Run II | CDF | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 100 |
| Lepton + jets | Run II | D0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 |
| Lepton + jets | Run I | CDF | 0 | 0 | 100 | 0 | 0 | 100 | 0 | 0 | 100 | 0 | 0 | 0 |


|  |  |  | $\begin{aligned} & \sqrt[1]{0} \\ & 0 \\ & \vdots \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0.0 \\ & 0 \end{aligned}$ | $\begin{aligned} & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \end{aligned}$ | $\begin{aligned} & \frac{1}{0} \\ & 0 \\ & \vdots \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \\ & 0 \end{aligned}$ | 8 <br> 0 <br> 0 <br> 0 <br> 0 <br> 0 <br> 0 <br> 0 <br> 0 <br> 0 <br> Cali |  <br> on <br> cor <br> In s |  | $\begin{aligned} & \stackrel{1}{0} \\ & 0 \\ & \vdots \\ & \vdots \\ & 0 \\ & 0 \\ & 0 \\ & 00 \\ & 00 \\ & 0 \end{aligned}$ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Lepton + jets | Run I | D0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 |
| Alljets | Run II | CDF | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 100 |
| Alljets | Run I | CDF | 0 | 0 | 100 | 0 | 0 | 100 | 0 | 0 | 100 | 0 | 0 | 0 |
| Dileptons | Run II | CDF | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 100 |
| Dileptons | Run II | D0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 |
| Dileptons | Run I | CDF | 0 | 0 | 100 | 0 | 0 | 100 | 0 | 0 | 100 | 0 | 0 | 0 |
| Dileptons | Run I | D0 | 0 | 0 | 0 | 100 | 0 | 0 | 0 | 0 | 0 | 100 | 0 | 0 |
| $\mathbb{E}_{T}+$ jets | Run II | CDF | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 100 |
| Decay length | Run II | CDF | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 100 |

## E. Measurement weights

As discussed in Sec. III A, the combined mass $m_{t}^{\text {comb }}$ is defined through the set of weights that minimize the squared difference between $m_{t}^{\text {comb }}$ and the true value of $m_{t}$, which is equivalent to minimizing the sum of the covariance matrix elements. Table V gives the weights $w_{i}$ for each of the input measurements as determined in this minimization. A weight of zero means that an input measurement has no effect on $m_{t}^{\text {comb }}$. The Run I measurement weights are negative, which reflects the fact that the correlations for these and other measurements are larger than the ratio of their total uncertainties [33]. In this case, the less precise measurement may acquire a negative weight. Input measurements with negative weights still affect the value of $m_{t}^{\text {comb }}$ and reduce the total uncertainty. By design, the sum of the weights is set to unity.

## IV. RESULTS OF THE COMBINATION

## A. Tevatron top-quark mass result

Combining the 12 independent measurements of $m_{t}$ from the CDF and D0 Collaborations yields

$$
\begin{aligned}
m_{t}^{\text {comb }} & =173.18 \pm 0.56(\text { stat }) \pm 0.75(\text { syst }) \mathrm{GeV} \\
& =173.18 \pm 0.94 \mathrm{GeV}
\end{aligned}
$$

The uncertainties are split into their components in Table II and Fig. 5. The jet energy scale contributes 0.49 GeV to the total systematic uncertainty. Of this, 0.39 GeV arises from limited statistics of the in situ JES calibration and 0.30 GeV
from the remaining contributions. Figure 6 summarizes the input $m_{t}$ values and the combined result.

We assess the consistency of the input $m_{t}$ measurements with their combination using a $\chi^{2}$ test statistic, defined as follows:

$$
\begin{aligned}
\chi_{\text {comb }}^{2}= & \left(\boldsymbol{m}_{\boldsymbol{t}}^{i}-\boldsymbol{m}_{\boldsymbol{t}}^{\text {comb }}\right)^{T} \text { Covariance }{ }^{-1} \\
& \times\left(m_{t}^{i}, m_{t}^{j}\right)\left(\boldsymbol{m}_{\boldsymbol{t}}^{j}-\boldsymbol{m}_{\boldsymbol{t}}^{\text {comb }}\right),
\end{aligned}
$$

where $\boldsymbol{m}_{t}^{i}$ is a column vector of the $12 m_{t}$ inputs, $\boldsymbol{m}_{\boldsymbol{t}}^{\text {comb }}$ is a matching column vector for the measurements adjusted in the previous minimization, and the superscript $T$ denotes the transpose. We find

$$
\chi_{\mathrm{comb}}^{2}=8.3 \text { for } 11 \text { degrees of freedom }
$$

which is equivalent to a $69 \%$ probability for agreement (i.e., $p$ value for the observed $\chi^{2}$ value) among the 12 input measurements.

## B. Consistency checks

We check one aspect of the assumption that biases in the input $m_{t}$ are on average zero (see Sec. III A) by calculating separately the combined $m_{t}^{\text {comb }}$ for each $t \bar{t}$ decay mode, each run period, and each experiment. The results are shown in Table VI. The resulting $m_{t}^{\text {comb }}$ values are calculated using all 12 input measurements and their correlations. The $\chi^{2}$ test statistic provides the compatibility of each subset with the others and is defined as
$\chi_{\mathrm{sub} 1, \mathrm{sub} 2}^{2},=\left(m_{t}^{\mathrm{sub} 1}-m_{t}^{\mathrm{sub} 2}\right)^{2}$ Covariance ${ }^{-1}\left(m_{t}^{\mathrm{sub} 1}-m_{t}^{\mathrm{sub} 2}\right)$.

TABLE IV. Correlations in systematic uncertainties (in percent) among the different measurements of $m_{t}$ (continued).

|  |  |  | Lepton + jets <br> Run II CDF | $\begin{aligned} & \text { Lepton + jets } \\ & \text { Run II D0 } \end{aligned}$ | Lepton + jets <br> Run I CDF | $\begin{aligned} & \text { Lepton + jets } \\ & \text { Run I D0 } \end{aligned}$ | Alljets <br> Run II CDF <br> Li | Alljets <br> Run I CDF <br> ht-jet response | Dileptons Run II CDF (1) (JES) | Dileptons Run II D0 | Dileptons <br> Run I CDF | Dileptons <br> Run I D0 | $\begin{gathered} \not \boldsymbol{t}_{T}+\text { jets } \\ \text { Run II CDF } \end{gathered}$ | Decay length Run II CDF |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Lepton + jets | Run II | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Lepton + jets | Run II | D0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 |
| Lepton + jets | Run I | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Lepton + jets | Run I | D0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 |
| Alljets | Run II | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Alljets | Run I | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Dileptons | Run II | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Dileptons | Run II | D0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 |
| Dileptons | Run I | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Dileptons | Run I | D0 | 0 | 100 | 0 | 100 | 0 | 0 | 0 | 100 | 0 | 100 | 0 | 0 |
| $E_{T}+$ jets | Run II | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Decay length | Run II | CDF | 100 | 0 | 100 | 0 | 100 | 100 | 100 | 0 | 100 | 0 | 100 | 100 |
| Out-of-cone correction (JES) |  |  |  |  |  |  |  |  | Model for $b$ | jets (JES) |  |  | Signal mode |  |
|  |  |  |  |  |  |  | 100\% correlated among all measurements |  |  |  |  |  |  |  |

TABLE V. Correlations in \% among the input $m_{t}$ measurements and their weights in the BLUE combination.

|  |  | Lepton + jets <br> Run II CDF | $\begin{gathered} \text { Lepton + jets } \\ \text { Run II D0 } \end{gathered}$ | Lepton + jets <br> Run I CDF | $\begin{gathered} \text { Lepton + jets } \\ \text { Run I D0 } \end{gathered}$ | $\begin{gathered} \text { Alljets } \\ \text { Run II CDF } \end{gathered}$ | Alljets <br> Run I CDF | Dileptons <br> Run II CDF | Dileptons <br> Run II D0 | Dileptons <br> Run I CDF | Dileptons Run I D0 | $\begin{gathered} \ddot{\not}_{T}+\text { jets } \\ \text { Run II CDF } \end{gathered}$ | Decay length <br> Run II CDF | Weight |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Lepton + jets | Run II CDF | 100 | 27 | 45 | 25 | 25 | 26 | 44 | 12 | 26 | 11 | 24 | 8 | 55.50 |
| Lepton + jets | Run II D0 | 27 | 100 | 21 | 14 | 16 | 9 | 11 | 39 | 13 | 7 | 15 | 6 | 26.66 |
| Lepton + jets | Run I CDF | 45 | 21 | 100 | 26 | 25 | 32 | 54 | 12 | 29 | 11 | 22 | 7 | -4.72 |
| Lepton + jets | Run I D0 | 25 | 14 | 26 | 100 | 12 | 14 | 27 | 7 | 15 | 16 | 10 | 5 | -0.06 |
| Alljets | Run II CDF | 25 | 16 | 25 | 12 | 100 | 15 | 25 | 10 | 15 | 7 | 14 | 4 | 13.99 |
| Alljets | Run I CDF | 26 | 9 | 32 | 14 | 15 | 100 | 38 | 6 | 19 | 7 | 14 | 4 | -0.80 |
| Dileptons | Run II CDF | 44 | 11 | 54 | 27 | 25 | 38 | 100 | 7 | 32 | 13 | 22 | 6 | 1.41 |
| Dileptons | Run II D0 | 12 | 39 | 12 | 7 | 10 | 6 | 7 | 100 | 8 | 5 | 10 | 3 | 2.28 |
| Dileptons | Run I CDF | 26 | 13 | 29 | 15 | 15 | 19 | 32 | 8 | 100 | 8 | 14 | 4 | -1.05 |
| Dileptons | Run I D0 | 11 | 7 | 11 | 16 | 7 | 7 | 13 | 5 | 8 | 100 | 6 | 2 | -0.15 |
| $\boldsymbol{E}_{T}+\mathrm{jets}$ | Run II CDF | 24 | 15 | 22 | 10 | 14 | 14 | 22 | 10 | 14 | 6 | 100 | 4 | 6.65 |
| Decay length | Run II CDF | 8 | 6 | 7 | 5 | 4 | 4 | 6 | 3 | 4 | 2 | 4 | 100 | 0.29 |



FIG. 6 (color online). The 12 input measurements of $m_{t}$ from the Tevatron collider experiments along with the resulting combined value of $m_{t}^{\text {comb }}$. The gray region corresponds to $\pm 0.94 \mathrm{GeV}$.

The $\chi^{2}$ values in Table VI show that biases in the input measurements are not large.

To check the impact of the assumption that the systematic uncertainty terms are either $0 \%$ or $100 \%$ correlated between input measurements, we change all off-diagonal $100 \%$ values to $50 \%$ (see Tables III and IV) and recalculate the combined top-quark mass. This extreme change shifts the central mass value up by 0.17 GeV and reduces the uncertainty negligibly. The chosen approach is therefore conservative.

## C. Summary

We have combined 12 measurements of the mass of the top quark by the CDF and D0 collaborations at the Tevatron collider and find

$$
m_{t}^{\text {comb }}=173.18 \pm 0.56(\text { stat }) \pm 0.75(\text { syst }) \mathrm{GeV}
$$

which corresponds to a precision of $0.54 \%$. The result is shown in Table VII together with previous combined results for comparison. The input measurements for this combination use up to $5.8 \mathrm{fb}^{-1}$ of integrated luminosity for each experiment, while $10 \mathrm{fb}^{-1}$ are now available. We therefore expect the final combination to improve in precision with the use of all the data, but also from analyzing all $t \bar{t}$ decay channels in both experiments and from the application of improved measurement techniques, signal and background models, and calibration corrections to all channels that will reduce systematic uncertainties. Currently, there are also some overlaps of the systematic effects that are included in different uncertainty categories.

TABLE VI. Separate calculations of $m_{t}^{\text {comb }}$ for each $t \bar{t}$ decay mode, by run period, and by experiment, and their $\chi^{2}$ probabilities.

| Subset | $m_{t}^{\text {comb }}$ | Consistency $\chi^{2}$ (Degrees of freedom $=1$ ) |  |  |  |  |  | $\begin{aligned} & \text { Lepton+ } \\ & \text { jets } \end{aligned}$ | $\chi^{2}$ probability |  |  |  | CDF-D0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $\begin{aligned} & \text { Lepton }+ \\ & \text { jets } \end{aligned}$ | Alljets | Dileptons | $\begin{gathered} \not \boldsymbol{E}_{T}+ \\ \text { jets } \end{gathered}$ | $\begin{gathered} \text { Run } \\ \text { II-Run I } \end{gathered}$ | CDF-D0 |  | Alljets | Dileptons | $\begin{gathered} \mathbb{E}_{T}+ \\ \text { jets } \end{gathered}$ | $\begin{gathered} \text { Run } \\ \text { II-Run I } \end{gathered}$ |  |
| Lepton + jets | $173.4 \pm 1.0$ | . . | 0.14 | 1.51 | 0.28 |  |  | $\ldots$ | 71\% | 22\% | 60\% |  |  |
| Alljets | $172.7 \pm 1.9$ | 0.14 | $\ldots$ | 0.40 | 0.04 |  |  | 71\% | $\cdots$ | 53\% | 85\% |  |  |
| Dileptons | $171.1 \pm 2.1$ | 1.51 | 0.40 | . . | 0.12 |  |  | 22\% | 53\% | ... | 73\% |  |  |
| $\mathbb{E}_{T}+$ jets | $172.1 \pm 2.5$ | 0.28 | 0.04 | 0.12 | . . |  |  | 60\% | 85\% | 73\% | . . |  |  |
| Run II | $173.6 \pm 1.0$ |  |  |  |  | 2.89 |  |  |  |  |  | 9\% |  |
| Run I | $180.0 \pm 4.1$ |  |  |  |  |  |  |  |  |  |  |  |  |
| CDF | $172.5 \pm 1.0$ |  |  |  |  |  | 2.56 |  |  |  |  |  | 11\% |
| D0 | $174.9 \pm 1.4$ |  |  |  |  |  |  |  |  |  |  |  |  |

TABLE VII. Mass measurements of the top quark from 1999 until this publication at the Tevatron collider.

| Year | Integrated luminosity $\left[\mathrm{fb}^{-1}\right]$ | $m_{t}[\mathrm{GeV}]$ | Uncertainty on $m_{t}$ | Reference |
| :---: | :---: | :---: | :---: | :---: |
| 1999 | 0.1 | $174.3 \pm 3.2 \pm 4.0$ | $2.9 \%$ | $[35]$ |
| 2004 | 0.1 | $178.0 \pm 2.7 \pm 3.3$ | $2.4 \%$ | $[36]$ |
| 2005 | 0.3 | $172.7 \pm 1.7 \pm 2.4$ | $1.7 \%$ | $[37]$ |
| 2006 | 0.7 | $172.5 \pm 1.3 \pm 1.9$ | $1.3 \%$ | $[38]$ |
| 2006 | 1.0 | $171.4 \pm 1.2 \pm 1.8$ | $1.2 \%$ | $[39]$ |
| 2007 | 2.1 | $170.9 \pm 1.1 \pm 1.5$ | $1.1 \%$ | $[40]$ |
| 2008 | 2.1 | $172.6 \pm 0.8 \pm 1.1$ | $0.8 \%$ | $[41]$ |
| 2008 | 2.1 | $172.4 \pm 0.7 \pm 1.0$ | $0.7 \%$ | $[42]$ |
| 2009 | 3.6 | $173.1 \pm 0.6 \pm 1.1$ | $0.7 \%$ | $[43]$ |
| 2010 | 5.6 | $173.32 \pm 0.56 \pm 0.89$ | $0.61 \%$ | $[44]$ |
| 2011 | 5.8 | $173.18 \pm 0.56 \pm 0.75$ | $0.54 \%$ | [45] |
|  | 5.8 | $173.18 \pm 0.56 \pm 0.75$ | $0.54 \%$ | This paper |

In addition to the in situ light-jet calibration systematic uncertainty that will scale down with the increase of analyzed luminosity, these levels of double counting are expected to be reduced for the next combination. The combination presented here has a $0.54 \%$ precision on $m_{t}$, making the top quark the particle with the best known mass in the SM.

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## APPENDIX A: EVALUATION OF SYSTEMATIC UNCERTAINTIES

Systematic uncertainties arise from inadequate modeling of signal and backgrounds and from the inability to reproduce the detector response with simulated events. Systematic uncertainties also arise from ambiguities in reconstructing the top quarks from their jet and lepton remnants. We minimize such uncertainties by using independent data to calibrate the absolute response of the detector, and we use state-of-the-art input from theory for
modeling the signal and backgrounds. We use alternative models for signal and different parameters for modeling backgrounds to check our assumptions.

Table VIII lists the uncertainties from the Run II lepton + jets measurements for CDF and D0 that are based on the matrix-element technique [24,25]. These two measurements provide most of the sensitivity to the combined $m_{t}$ result and are discussed below. Before explaining how each individual systematic uncertainty is estimated, we will first discuss how the uncertainties from different sources are propagated to $m_{t}$ and how they are calculated using ensembles of pseudoexperiments.

Uncertainties related to the performance of the detector and calibration of the reconstructed objects, such as JES, the modeling of jets, leptons, and triggers, and calibration of the $b$-tagging algorithms, are evaluated by shifting the central values of their respective parameters by $\pm 1$ standard deviations $(\sigma)$ that correspond to the uncertainties on each value. This is done using MC $t \bar{t}$ events for $m_{t}=$ 172.5 GeV . The integrations over the matrix element are performed again for each shifted sample and define shifts in $m_{t}$ that correspond to each independent source of systematic uncertainty. These uncertainties are not determined at other $m_{t}$ values, and it is assumed that their dependence on $m_{t}$ is minimal.

For uncertainties that arise from ambiguities in the modeling of the $t \bar{t}$ signal, which include the uncertainties from initial- and final-state radiation, higher-order QCD corrections, $b$-jet hadronization, light-jet hadronization, the underlying-event model, and color reconnection, we generate simulated $t \bar{t}$ events using alternative models also at $m_{t}=172.5 \mathrm{GeV}$. These events are processed through detector simulation and are reconstructed, and the probability density is calculated by integration over the matrix elements.

For the uncertainties from the choice of parton distribution functions, the ratio of contribution from quark annihilation and gluon fusion, and models for overlapping

TABLE VIII. Individual components of uncertainty on CDF and D0 $m_{t}$ measurements in the lepton + jets channel for Run II data [24,25].

| Systematic | Uncertainty [GeV] |  |
| :---: | :---: | :---: |
|  | CDF ( $5.6 \mathrm{fb}^{-1}$ ) | D0 (3.6 fb ${ }^{-1}$ ) |
| Source | $m_{t}=173.00 \mathrm{GeV}$ | $m_{t}=174.94 \mathrm{GeV}$ |
| DETECTOR RESPONSE |  |  |
| Jet energy scale |  |  |
| Light-jet response (1) | 0.41 | n/a |
| Light-jet response (2) | 0.01 | 0.63 |
| Out-of-cone correction | 0.27 | n/a |
| Model for $b$ jets | 0.23 | 0.07 |
| Semileptonic b decay | 0.16 | 0.04 |
| $b$-jet hadronization | 0.16 | 0.06 |
| Response to $b / q / g$ jets | 0.13 | 0.26 |
| In situ light-jet calibration | 0.58 | 0.46 |
| Jet modeling | 0.00 | 0.36 |
| Jet energy resolution | 0.00 | 0.24 |
| Jet identification | 0.00 | 0.26 |
| Lepton modeling | 0.14 | 0.18 |
| MODELING SIGNAL |  |  |
| Signal modeling | 0.56 | 0.77 |
| Parton distribution functions | 0.14 | 0.24 |
| Quark annihilation fraction | 0.03 | n/a |
| Initial and final-state radiation | 0.15 | 0.26 |
| Higher-order QCD corrections | n/a | 0.25 |
| Jet hadronization and underlying event | 0.25 | 0.58 |
| Color reconnection | 0.37 | 0.28 |
| Multiple interactions model | 0.10 | 0.05 |
| MODELING BACKGROUND |  |  |
| Background from theory | 0.27 | 0.19 |
| Higher-order correction for heavy flavor | 0.03 | 0.07 |
| Factorization scale for $W+$ jets | 0.07 | 0.16 |
| Normalization to predicted cross sections | 0.25 | 0.07 |
| Distribution for background | 0.07 | 0.03 |
| Background based on data | 0.06 | 0.23 |
| Normalization to data | 0.00 | 0.06 |
| Trigger modeling | 0.00 | 0.06 |
| $b$-tagging modeling | 0.00 | 0.10 |
| Signal fraction for calibration | n/a | 0.10 |
| Impact of multijet background on the calibration | n/a | 0.14 |
| METHOD OF MASS EXTRACTION |  |  |
| Calibration method | 0.10 | 0.16 |
| STATISTICAL UNCERTAINTY | 0.65 | 0.83 |
| UNCERTAINTY ON JET ENERGY SCALE | 0.80 | 0.83 |
| OTHER SYSTEMATIC UNCERTAINTIES | 0.67 | 0.94 |
| TOTAL UNCERTAINTY | 1.23 | 1.50 |

interactions, we reweight the fully reconstructed simulated $t \bar{t} \mathrm{MC}$ events at $m_{t}=165,170,172.5,175$, and 180 GeV to reflect the uncertainty on the $\pm 1 \sigma$ range on each parameter and extract its impact on $m_{t}$.

Each method used to measure $m_{t}$ is calibrated using $t \bar{t}$ MC events generated at $m_{t}=165,170,172.5,175$, 180 GeV , which provide the relationship between input and "measured" masses. A straight line is fitted to these
values, representing a response function that is used to correct the $m_{t}$ measurement in data.

Systematic uncertainties are evaluated using studies of ensembles of pseudoexperiments. For each of the shifted or reweighted sets of events, and those based on alternative models or different generated $m_{t}$, we create an ensemble of at least 1000 pseudoexperiments, by means of binomially smeared signal and background fractions that match the
expectation in the data sample and with the total number of events in each pseudoexperiment equal to the number of events observed in data. We use the ensembles of such pseudoexperiments to assess the difference between generated and measured mass and to calibrate the method of mass extraction.

For the uncertainty on background, we change the fraction of background events in the pseudoexperiments within their uncertainties and remeasure the top-quark mass.

For the BLUE combination method, the uncertainties must be defined symmetrically around the central mass value, and this requirement determines part of the following definitions of uncertainty.

For the uncertainties obtained in ensemble studies with shifted or reweighted parameters, $m_{t}^{+}$corresponds to the $+1 \sigma$ shift in the input parameter and $m_{t}^{-}$corresponds to the $-1 \sigma$ shift. The systematic uncertainty on the value of $m_{t}$ from these parameters is defined as $\pm\left|m_{t}^{+}-m_{t}^{-}\right| / 2$, unless both shifts are in the same direction relative to the nominal value, in which case the systematic uncertainty is defined as the larger of $\left|m_{t}^{+}-m_{t}\right|$ or $\left|m_{t}^{-}-m_{t}\right|$.

For the values obtained from a comparison between two or more models, the systematic uncertainty is taken as $\pm$ of the largest difference among the resulting masses (without dividing by two).

## 1. Jet energy scale

The following seven terms (1.1-1.7) refer to the jet energy scale.

## a. Light-jet response (1)

This uncertainty includes the absolute calibration of the CDF JES for Run I and Run II and the smaller effects on JES from overlapping interactions and the model for the underlying event.

CDF's calibration of the absolute jet energy scale uses the single-pion response to calibrate jets in data and to tune the model of the calorimeter in the simulation. Uncertainties of these processes form the greatest part of the JES uncertainty. Small constant terms are added to account for the model of jet fragmentation and for calorimeter simulation of electromagnetically decaying particles, and to take into account small variations of the absolute calorimeter response over time. The total resulting uncertainty on the absolute JES is $1.8 \%$ for 20 GeV jets rising to $2.5 \%$ for 150 GeV jets.

At high Tevatron instantaneous luminosities, more than one $p \bar{p}$ interaction occurs during the same bunch crossing, and the average number of interactions depends linearly on instantaneous luminosity and is changed from $\approx 1$ to 8 between the start and the end of Run II. If the final-state particles from these extra $p \bar{p}$ interactions overlap with the jets from a $t \bar{t}$ event, the energy of these jets is increased, thereby requiring the correction. The uncertainty on this correction depends on vertex-reconstruction efficiency and
the rate for misidentifying vertices. The impact of these effects is checked on data samples, including $W \rightarrow e \nu$, minimum bias, and multijet events with a trigger threshold of 100 GeV . CDF finds an uncertainty of 0.05 GeV per jet. This uncertainty was estimated early in Run II. With increasing instantaneous luminosity, this correction was insufficient, and another systematic uncertainty term was introduced through the "multiple-interactions-model" term, which is described later.

CDF includes the impact of the underlying event on JES in this component of uncertainty. The proton and antiproton remnants of the collision deposit energy in the calorimeter, and these can contribute to the energy of the jets from $t \bar{t}$ decay, which must be subtracted before $m_{t}$ can be measured accurately. CDF compares the "Tune A" underlying-event model [71] in PYTHIA [66] with the JIMMY model $[84,85]$ in HERWIG [86] using isolated tracks with $p_{T}>0.5 \mathrm{GeV}$. The data agree well with Tune A, which is expected since it was tuned to CDF data, but differ from JIMMY by about $30 \%$. This difference is propagated to the absolute calibration of JES and yields a $2 \%$ uncertainty for low- $p_{T}$ jets and less than $0.5 \%$ for 35 GeV jets.

MC $t \bar{t}$ events are generated by CDF with jet energies shifted by the above three uncertainties, and the resulting shifts in $m_{t}$ are used to estimate the uncertainty. The overall uncertainty on $m_{t}$ from these combined sources is $0.24 \%$ for lepton + jets, $0.22 \%$ for alljets, $1.18 \%$ for CDF Run II dilepton data, and $0.26 \%$ for $\mathscr{Z}_{T}+$ jets for Run II data of CDF.

## b. Light-jet response (2)

This uncertainty term represents almost all parts of D0 Run I and Run II calibrations of JES. The absolute energy scale for jets in data is calibrated using $\gamma+$ jet data with photon $p_{T}>7 \mathrm{GeV}$ and $\left|\eta_{\gamma}\right|<1.0$, and jet $p_{T}>15 \mathrm{GeV}$ and $\left|\eta_{\text {jet }}\right|<0.4$, using the " $E_{T}$ projection fraction" method [82]. Simulated samples of $\gamma+$ jets and $Z+$ jets events are compared to data and used to correct the energy scale for jets in MC events. The JES is also corrected as a function of $\eta$ for forward jets relative to the central jets using $\gamma+$ jets and dijets data. Out-of-cone particle scattering corrections are determined with $\gamma+$ jets data and simulated events, without using overlays of underlying events, to avoid double counting of this effect. Templates of deposited energy are formed for particles belonging to and not belonging to a jet using 23 annular rings around the jet axis for $\mathcal{R}(y, \phi)=\sqrt{(\Delta y)^{2}+(\Delta \phi)^{2}} \leq 3.5$. All of these calibration steps are combined, and the total uncertainty on JES is calculated for light jets and heavy-flavor jets (independent of the type of jet). The resulting D0 uncertainty on $m_{t}$ for Run II lepton + jets events is $0.36 \%$ and $0.86 \%$ for dilepton data.

This uncertainty term also includes the relative jet energy correction as a function of jet $\eta$ for CDF. This is
measured using dijet data, along with PYTHIA and HERWIG simulations of $t \bar{t}$ events generated with shifted jet energies, and lead to the following uncertainties on Run II measurements of $m_{t}: 0.01 \%$ for lepton + jets, $0.02 \%$ for alljets, $0.34 \%$ for dileptons, and $0.03 \%$ for $\mathbb{E}_{T}+$ jets.

## c. Out-of-cone corrections

For all CDF measurements and for D0 Run I, this uncertainty component accounts for energy lost outside the jet reconstruction cone and uses the difference between two models of light-quark and gluon fragmentation and simulation of the underlying event. D0 changed the way it measures the out-of-cone uncertainty between Run I and Run II, and this uncertainty for D0 Run II measurements is therefore included in the light-jet response (2) term, described previously.

Energy is lost from the cone of jet reconstruction when a quark or gluon is radiated at a large angle relative to the original parton direction, or when the fragmentation shower is wider than the cone, or when low momentum particles are bent out of the cone by the axial magnetic field of the detector. Energy is gained in the cone from initialstate radiation and from remnants of spectator partons, called collectively at CDF the underlying event. The two models compared by CDF in Run II are PYTHIA with Tune A for the underlying event and HERWIG with the JIMMY modeling of the underlying event. For the narrow cone size of $\mathcal{R}=0.4$ used in measurements of $m_{t}$, more energy is lost from the cone than gained. The correction is measured using PYTHIA dijet events and data in the region $0.4<$ $\mathcal{R} \leq 1.3$. A small constant is added to compensate for energy outside the $\mathcal{R}>1.3$ region ("splash out"). The correction is largest for jets at low transverse momentum: $+18 \%$ for $p_{T}=20 \mathrm{GeV}$ jets and $<4 \%$ for jets with $p_{T}>$ 70 GeV . A detailed description of the method can be found in Ref. [81].

The uncertainty on these corrections is measured by comparing $\gamma+$ jets data to the two simulations. The largest difference between either of the models and data is taken as the uncertainty (the difference between the two models is very small). For jets with $p_{T}=20 \mathrm{GeV}$, the uncertainty on the jet energy scale is $6 \%$, and for jets above 70 GeV , it is $1.5 \%$. These translate into uncertainties on CDF Run II $m_{t}$ measurements of $0.16 \%$ for the lepton + jets measurement, $0.14 \%$ for alljets, $1.25 \%$ for dileptons, and $0.12 \%$ for $\boldsymbol{E}_{T}+$ jets.

## d. Energy offset

This uncertainty term is specific to D0 Run I measurements. It includes the uncertainty arising from uranium decays noise in the calorimeter and from the correction for multiple interaction to JES. These lead to uncertainties in $m_{t}$ of $0.72 \%$ for lepton + jets and $0.77 \%$ for dilepton events. In Run II, the integration time for the calorimeter electronics is short, after the upgrade to shorter
bunch-crossing time ( $3.5 \mu$ s to 396 ns ). This effect results in a negligible uncertainty on the offset for D0 Run II measurements of $m_{t}$.

## e. Model for b jets

(i) Semileptonic b decay

The uncertainty on the semileptonic branching fraction ( $10.69 \pm 0.22$ ) $\times 10^{-2}$ (PDG 2007 values) of $B$ hadrons affects the value of $m_{t}$. Both collaborations reweight $t \bar{t}$ events by $\pm$ the uncertainty on the central value ( $\pm 2.1 \%$ ) and take half the resulting mass difference as the uncertainty on $m_{t}: 0.09 \%$ for CDF and $0.03 \%$ for D0.
(ii) $b$-jet hadronization

For its nominal $m_{t}$ measurements, CDF uses the default PYTHIA model of $b$-jet fragmentation based on the Bowler model [87] ( $r_{q}=1.0, a=0.3, b=$ 0.58), where $r_{q}$ is the Bowler fragmentationfunction parameter and $a$ and $b$ are Lund fragmentation-function parameters. D0 uses a model with these parameters tuned to data from ALEPH, DELPHI, and OPAL [88] ( $r_{q}=0.897 \pm$ $0.013, a=1.03 \pm 0.08, b=1.31 \pm 0.08)$. To measure the uncertainty on these models, CDF compares its $m_{t}$ values to those measured with the LEP parameters used by D0 and to those from the SLD experiment at SLC [88] ( $r_{q}=0.980 \pm 0.010, a=$ $1.30 \pm 0.09, b=1.58 \pm 0.09)$. D0 compares the measured $m_{t}$ with the LEP parameters to the one from SLC. The resulting uncertainties on the $m_{t}$ extracted from the lepton + jets channel are $0.09 \%$ for CDF and $0.03 \%$ for D0.
For some analyses, the determination of the uncertainties in (i) and (ii) may be affected by statistical fluctuations of the MC samples.

## f. Response to $b / q / g$ jets

The calibrations of JES described in the first two paragraphs of the Appendix are derived on samples dominated by "light-quark" and gluon jets and applied to all jets. However, the calorimeter response to heavy-flavor jets differs in that these particles often decay semileptonically, and the $b$ jet will have some energy lost through the escaping neutrino. Bottom quark jets can also contain an electron that showers in a pattern different than for hadronic particles, or the jet may contain a muon that neither produces a shower nor gets absorbed in the calorimeter. Bottom jets also differ from light jets in the distribution of their shower and particle content. Since every $t \bar{t}$ event contains two $b$ jets, it is important to understand their energy calibration after the application of the previous overall corrections.

CDF measures an uncertainty from the difference between the $b$-jets response and light-flavor jets response in

Run II. CDF takes sets of MC $t \bar{t}$ events and cluster particles into jets classifying each such particle jet as a $b$ jet or a light jet [79]. Single-particle response for data and for MC events are applied to the formed particle jets to predict the energy measured in the calorimeter. A double ratio is calculated: $\left(p_{T}^{\text {data }} / p_{T}^{\mathrm{MC}}\right)_{b j \text { jets }} /\left(p_{T}^{\text {data }} / p_{T}^{\mathrm{MC}}\right)_{\text {lightjets }}$, which is found to be 1.010. The uncertainty on $m_{t}$ is measured by generating new $t \bar{t}$ samples with the $b$-jet scale shifted by this $1 \%$ difference, which results in $0.1 \%$ uncertainty in $m_{t}$ for the lepton + jets measurement.

For Run II measurements, D0 corrects the transversemomentum distributions of jets differently in four regions of detector pseudorapidity to make the MC response match that in data (after the main JES calibration) as a function of jet flavor: $b$ jets, light-quark jets $(u, d, s, c)$, and gluon jets [25]. The correction functions are shifted up and down by their uncertainties, and the extracted shifts in $m_{t}$ are used to define the resulting uncertainty on $m_{t}$ of $0.15 \%$ for the lepton + jets measurement and $0.23 \%$ for the dilepton measurement.

## g. In situ light-jet calibration

In $t \bar{t}$ events where one or both $W$ bosons decay to $q \bar{q}^{\prime}$, the world average value of $M_{W}$ [7] is used to constrain the jet energy scale for light-quark jets in situ [89,90]. CDF and D0 perform simultaneous measurements of $m_{t}$ and $M_{W}$, and fit a linear function to the JES for light-quark jets that is applied to all the jets to improve precision of $m_{t}$.

CDF measures the in situ rescaling factor independently in their lepton + jets, alljets, and $\mathscr{E}_{T}+$ jets analyses, and so these terms are uncorrelated. D0 applies the rescaling derived from their lepton + jets measurement to dilepton events, and these uncertainties are therefore correlated.

The uncertainty from the in situ calibration is determined through a two-dimensional minimization of a likelihood that is a function of top-quark mass and JES. The extracted JES is then shifted relatively to its measured central value, and a one-dimensional fit is performed to the top-quark mass. The difference in quadrature between the uncertainty on $m_{t}$ from the first and second fits is taken as the uncertainty on $m_{t}$ from the in situ calibration, giving $0.34 \%$ for CDF's lepton + jets measurement, $0.27 \%$ for D0's lepton + jets result, $0.55 \%$ for CDF's alljets, $0.89 \%$ for their $\not_{T}+$ jets measurement, and $0.32 \%$ for D0's dilepton measurement.

## 2. Jet modeling

Applying jet algorithms to MC events, CDF finds that the resulting efficiencies and resolutions closely match those in data. The small differences propagated to $m_{t}$ lead to a negligible uncertainty of 0.005 GeV , which is then ignored. D0 proceeds as follows.
(i) Jet energy resolution

The modeling of the jet energy resolution is corrected in D 0 to match that in data. The value of $m_{t}$
is then remeasured using MC samples with jet energy resolution corrections shifted up and down by their uncertainties, resulting in an uncertainty on $m_{t}$ of $0.18 \%$.
(ii) Jet identification

D0 applies correction functions to MC events to match the jet identification efficiency in data. The uncertainty on $m_{t}$ is estimated by reducing the corrections by $1 \sigma$ and remeasuring the mass in the adjusted MC samples. The efficiency can only be shifted down and not up because jets can be removed from the simulated events but not added. The uncertainty on $m_{t}$ is therefore set to $\pm$ the single-sided shift and is $0.15 \%$.

## 3. Lepton modeling

(i) Momentum scale for leptons

In Run II, the electron and muon channels for CDF and the muon channels for D0 are used to calibrate the lepton momentum scales by comparing the invariant dilepton mass $m_{\ell 1 \ell 2}=$ $\sqrt{\left(E_{\ell 1}+E_{\ell 2}\right)^{2}-\left(p_{\ell 1}+p_{\ell 2}\right)^{2}}$ for $J / \psi \rightarrow \ell \ell$ and $Z \rightarrow \ell \ell$ decays in MC events with data. The positions of the resonances observed in the $m_{\ell \ell}$ distributions reflect the absolute momentum scales for the leptons. CDF and D0 perform a linear fit as a function of the mean value of transverse momentum to the two mass points $(3.0969 \mathrm{GeV}$ and 91.1876 GeV [7]), assuming that any mismatch is attributable to an uncertainty in the calibration of the magnetic field. D0 also fits a quadratic relation, assuming that the difference in scale arises from misalignment of the detector. The value of $m_{t}$ is measured using MC $t \bar{t}$ ensembles without rescaling lepton $p_{T}$ and with lepton $p_{T}$ values rescaled using these fitted relations. Half of the largest difference in extracting $m_{t}$ is taken as its systematic uncertainty resulting from the lepton $p_{T}$ scale. For muon measurements from D0, the largest shift is observed for the linear parametrization. In Run I, this source of uncertainty was neglected as it was negligible relative to other sources of uncertainty.
In D0 Run II measurement of the $W$-boson mass in the electron decay channel, it was found that 0.26 radiation length of material was left out in the GEANT modeling of the solenoid [91]. The Z-boson mass peak was used to calculate a quadratic correction to the electron energy by comparing MC events generated with additional solenoid material to data. This correction was then propagated to the $m_{t}$ measurement.
The uncertainties on the $m_{t}$ measurements from the lepton momentum scale are $0.08 \%$ for CDF lepton + jets measurements and $0.10 \%$ for D0, and $0.16 \%$ for

CDF dilepton measurements and $0.28 \%$ for D0 dilepton results.
(ii) Lepton momentum resolution

The muon momenta in simulated events at D0 are smeared to match the resolution in data. The uncertainty on this correction corresponds to an uncertainty on $m_{t}$ of $0.17 \%$.

## 4. Signal modeling

(i) Parton distribution functions

In Run I, the uncertainties from choice of PDF are determined by measuring the change in $m_{t}$ using the MRSA' set [92] instead of $\mathrm{MRSD}_{0}^{\prime}$ [62] or CTEQ4M [63], and are found to be negligible.
In Run II, the uncertainty is measured by CDF by comparing CTEQ5L results with MRST98L [93], by changing the value of $\alpha_{s}$ in the MRST98L model, and by varying the 20 eigenvectors in CTEQ6M [69]. The total uncertainty is obtained by combining these sources in quadrature. D0 measures this uncertainty by reweighting the PYTHIA model to match possible excursions in the parameters represented by the 20 CTEQ6M uncertainties and taking the quadratic sum of the differences. The resulting uncertainty on $m_{t}$ is $0.08 \%$ for CDF and $0.14 \%$ for D0.
(ii) Fractional contributions from quark annihilation and gluon fusion
In Run I, this source of uncertainty in $t \bar{t}$ production is not considered. In Run II, CDF estimates the effect on $m_{t}$ by reweighting the gluon fusion fraction in the PYTHIA model from 5\% to $20 \%$ [94]. The uncertainty on $m_{t}$ is found to be $0.02 \%$. This uncertainty is included by D 0 in the systematic component (iv) below, where the effects of higher-order QCD corrections are discussed.
(iii) Initial- and final-state radiation

Initial- and final-state radiation refers to additional gluons radiated from the incoming or outgoing partons or from the top quarks. Jets initiated by these gluons affect the measured value of $m_{t}$ because they can be misidentified as jets from the final-state partons in top-quark decay. Extensive checks were performed in Run I measurements to assess the effects of initial and final-state radiation by varying parameters in HERWIG.
In Run II, uncertainties from initial- and final-state radiation are assessed by both collaborations using a CDF measurement [95] in Drell-Yan dilepton events that have the same $q \bar{q}$ initial state as most $t \bar{t}$ events, but no final-state radiation. The mean $p_{T}$ of the produced dilepton pairs is measured as a function of the dilepton invariant mass, and the values of $\Lambda_{\mathrm{QCD}}$ and the $Q^{2}$ scale in the MC that matches best the data when extrapolated to the $t \bar{t}$
mass region are found. CDF's best-fit values are $\Lambda_{\mathrm{QCD}}(5$ flavors $)=292 \mathrm{MeV}$ with $0.5 \times Q^{2}$ and $\Lambda_{\mathrm{QCD}}(5$ flavors $)=73 \mathrm{MeV}$ with $2.0 \times Q^{2}$ for $\pm \sigma$ excursions around the mean dilepton $p_{T}$ values. Since the initial- and final-state shower algorithms are controlled by the same QCD evolution equation [64], the same variations of $\Lambda_{\mathrm{QCD}}$ and $Q^{2}$ scale are used to estimate the effect of final-state radiation. The resulting uncertainty for modeling of the initial- and final-state radiation is $0.09 \%$ for CDF and $0.15 \%$ for D0. The correction algorithm does not distinguish between "soft" (out-of-cone) and "hard" (separate jet) radiation, and there is therefore some overlap between the uncertainty on $m_{t}$ for the out-of-cone jet energy correction and for gluon radiation. There is also some overlap between the uncertainty for initial- and final-state radiation and the uncertainty on higher-order QCD corrections for high- $p_{T}$ radiation.
(iv) Higher-order QCD corrections

Higher-order QCD corrections to $t \bar{t}$ production are not used for Run I measurements, as only LO generators were available at that time. D0 measures higher-order jet-modeling uncertainties in Run II by comparing $m_{t}$ extracted with ALPGEN and HERWIG for evolution and fragmentation to the value obtained from events generated with MC@NLO [96], which uses HERWIG parton showering with a NLO model for the hard-scattering process. This component of uncertainty also includes (for D0) the uncertainty from the fraction of quark-antiquark to gluon-gluon contributions to the initial state. CDF also studies differences in $m_{t}$ using MC@NLO and finds that the uncertainties in distributions in the number of jets and the transverse momentum of the $t \bar{t}$ system overlap with the uncertainty from initialand final-state radiation. Future measurements of $m_{t}$ are expected to treat these uncertainties separately. The uncertainty on $m_{t}$ from higher-order contributions and initial-state $q \bar{q} / g g$ ratio is $0.14 \%$ for D 0 .
(v) Jet hadronization and underlying event

In Run I, CDF measured the uncertainty in the model for parton showering and hadronization and the underlying event by comparing the value of $m_{t}$ based on HERWIG to that on PYTHIA [97], and D0 compared HERWIG results to those from ISAJET [98]. In Run II, CDF estimates these uncertainties by comparing $m_{t}$ obtained using PYTHIA with Tune A of the underlying-event model to results from HERWIG with a tuned implementation of the underlying-event generator JIMMY. D0 estimates these uncertainties by comparing identical sets of hard-scatter events from ALPGEN coupled to HERWIG instead of to PYTHIA. For the uncertainty on $m_{t}$, this corresponds to $0.40 \%$ for CDF and $0.33 \%$ for D0.
(vi) Color reconnection

There are up to six final-state quarks in $t \bar{t}$ events, in addition to initial- and final-state radiation. When hadronization and fragmentation occur, there are color interactions among these partons and the color remnants of the proton and antiproton. This process is referred to as "color reconnection." It changes the directions and distributions of finalstate jets $[99,100]$, which affects the reconstructed value of $m_{t}$ [72].
The uncertainty on color reconnection was not evaluated for Run I because appropriate MC tools were not available at that time. Both collaborations estimate this effect in Run II by comparing the value of $m_{t}$ extracted from ensembles of $t \bar{t}$ events generated by PYTHIA using the difference between two parton shower simulations: (i) angular ordering for jet showers (same as used in the nominal $m_{t}$ measurements) using the A-PRO underlying-event model (Tune A but updated using the "Professor" tuning tool [101]), and (ii) ACR-PRO. ACR-PRO is identical to A-PRO except that it includes color reconnection in the model. The resulting uncertainties on $m_{t}$ are $0.32 \%$ for CDF and $0.16 \%$ for D0.

## 5. Multiple interactions model

Monte Carlo simulated events are overlaid with Poissondistributed low- $p_{T}$ events (PYTHIA MC events for CDF, "zero-bias" data for D0) to simulate the presence of simultaneous additional $p \bar{p}$ interactions. The mean number of overlaid events is chosen at the time of event generation, but in data, the number of such interactions changes with instantaneous luminosity of the Tevatron.

CDF measures $m_{t}$ as a function of the number of multiple interactions, finding a change of $0.07 \pm 0.10 \mathrm{GeV}$ per primary vertex. For CDF's measurements, the average number of primary vertices in data is 2.20 and for simulated events it is 1.85 , leading to an uncertainty on $m_{t}$ of $0.02 \%$. CDF adds to this in quadrature a term to cover the difference in jet energy response as a function of the number of multiple interactions of $0.06 \%$, giving a total uncertainty of $0.06 \%$.

D0 reweights the simulated events to make the instantaneous luminosity distribution match that in data. The resulting uncertainty on $m_{t}$ is $0.03 \%$.

## 6. Background from theory

(i) Higher-order correction for heavy flavor

D0 corrects the leading-log $W+$ jets cross section from ALPGEN to NLO precision before normalizing this background to data. This increases the fraction of $W b \bar{b}$ and $W c \bar{c}$ events in $W+$ jets by a factor of $1.47 \pm 0.50$. CDF normalizes the $W+$ heavy-flavor jets background to data independent of the other
components in $W+$ jets, which has a similar effect. The resulting uncertainties on $m_{t}$ are $0.11 \%$ for CDF and $0.04 \%$ for D0.
(ii) Factorization scale for $W+$ jets

The transverse momenta of the jets in $W+$ jets events are sensitive to the factorization and renormalization scales chosen for the calculations. These two scales are set equal to each other, with $Q^{2}=$ $M_{W}^{2}+\sum p_{T}^{2}$. To determine the uncertainty on $m_{t}$, the scale is changed from $(Q / 2)^{2}$ to $(2 \times Q)^{2}$, the MC events regenerated, and the mass remeasured. Changing the scale does not affect the fraction of $W+$ jets in the model but does affect the transversemomentum distributions of the jets. The uncertainties on $m_{t}$ are $0.02 \%$ for CDF and $0.09 \%$ for D0.
(iii) Normalization to predicted cross sections

CDF divides the background into seven independent parts: $W+$ heavy-flavor jets, $W+$ light-flavor jets, single-top $t q b$ and $t b, Z+$ jets, dibosons ( $W W, W Z$, and $Z Z$ ), and multijet contributions. This uncertainty term covers the normalization of the components modeled with MC simulated events (not multijets). The small backgrounds from single-top, $Z+$ jets, and diboson production are normalized to NLO calculations. The uncertainties on the cross sections are $10 \%$ for $t q b, 12 \%$ for $t b, 14 \%$ for $Z+$ jets, and $10 \%$ for dibosons. The $W+$ jets background is normalized to data before implementation of $b$ tagging, using a fit to the distribution for $\mathbb{E}_{T}$ in the event. The uncertainty on this normalization cannot easily be disentangled from the other sources, and so it is kept in this category. The combined uncertainty on $m_{t}$ from these normalizations is $0.09 \%$.
D0 also normalizes single-top, $Z+$ jets, and diboson contributions, in all analysis channels, and Drell-Yan in the dilepton channel, to next-to-leading-order cross sections, using values from the MCFM event generator [102]. The uncertainties on the cross sections take into account the uncertainty on th ePDF and on the choice of factorization and renormalization scales, which together propagate through to $m_{t}$ an uncertainty of $0.04 \%$.
(iv) Background differential distributions

For CDF, different methods were used to estimate the uncertainty attributable to the overall background shape. In the recent lepton + jets analysis, this uncertainty was assessed by dividing randomly the background events into subsets, building the background likelihood from one of the subsets, and reconstructing the $m_{t}$ from the second subset. In the next step, the difference in $m_{t}$ obtained from the second subset and the nominal $m_{t}$ value is evaluated. This contributes an uncertainty of $0.03 \%$. CDF also estimates an uncertainty from
the limited MC statistics used to measure the background. This yields an additional $0.03 \%$ uncertainty on $m_{t}$.
For D0, the $p_{T}$ and $\eta$ distributions of jets in $W+$ jets events do not fully reproduce those in data. An uncertainty to cover these deviations is based on the difference between the model for background and data in the $\eta$ distribution of the third jet in three-jet events. The resultant uncertainty on $m_{t}$ is $0.09 \%$.

## 7. Background based on data

(i) Normalization to data

In the lepton + jets, alljets, $\mathscr{E}_{T}+$ jets, and decaylength channels, backgrounds from multijet events are normalized to data. In the lepton + jets analyses at D 0 , the $W+$ jets background model is combined with the contribution from multijet events, and both are normalized simultaneously to data, so that their uncertainties in normalization are anticorrelated. In dilepton analyses at CDF, the Drell-Yan background is normalized to data. For the lepton + jets analyses, CDF uncertainty on $m_{t}$ from the normalization of the multijet backgrounds to data is $0.03 \%$, and D0's uncertainty for the normalization of $W+$ jets and multijets to data is $0.13 \%$.
(ii) Trigger modeling

CDF expects a negligible uncertainty on $m_{t}$ from the modeling of the trigger. D0 simulates the trigger turn-on efficiencies for MC events by applying weights as a function of the transverse momentum of each object in the trigger. The uncertainty is measured by setting all the trigger efficiencies to unity and recalculating the value of $m_{t}$, which shifts $m_{t}$ by $0.03 \%$.
(iii) $b$-tagging modeling

CDF applies the $b$-tagging algorithm directly to MC events and finds that any difference between the $b$-tagging behavior in MC and data has a negligible impact on the measurement of $m_{t}$. D0 applies the $b$-tagging algorithm directly to

MC events for recent Run II measurements. Previously $b$-tagging was simulated with tag probability, and in Run I, as D0 did not have a silicon tracker, nonisolated muons were used to identify $b$ jets. The tagging efficiency for simulated events is made to match that in data by randomly dropping $b$ tags for $b$ and $c$ jets, while assigning a per jet weight for tagging light-flavor jets as $b$ jets. The uncertainties for these corrections are determined by shifting the efficiencies for tagging $b$ and $c$ jets by $5 \%$ and by $20 \%$ for light jets, which introduces an uncertainty on $m_{t}$ of $0.06 \%$.
(iv) Signal fraction for calibration

D0 measures the impact of the uncertainty in the ratio of signal to background events, which affects the calibration of $m_{t}$. Changing the signal fraction within uncertainty results in an uncertainty on $m_{t}$ of $0.06 \%$.
(v) Impact of multijet background on the calibration Multijet background events are not used in D0 samples that determine the calibration of $m_{t}$ for the lepton + jets measurement since the background probability for such events is much larger than the signal probability. The assumption that this has a small effect on $m_{t}$ is tested by selecting a multijetenriched sample of events from data (by inverting the lepton isolation criteria) and adding these events when deriving the calibration. Applying this alternative calibration to data indicates that $m_{t}$ can shift by an uncertainty of $0.08 \%$.

## 8. Calibration method

Monte Carlo $t \bar{t}$ ensembles are generated at different values of input $m_{t} \quad\left(m_{t}=165,170,172.5,175\right.$, 180 GeV ), and calibrations relate the input masses for $t \bar{t}$ events to the extracted masses using a straight line. For some of the $m_{t}$ measurements, there is an additional in situ calibration of the JES to the light quarks in $W$-boson decay, which is then applied to all jets. The uncertainties from both calibrations are propagated to the uncertainty on $m_{t}$, which for CDF are $0.04 \%$ and $0.05 \%$, respectively, giving a total of $0.06 \%$. For D0, the uncertainty on $m_{t}$ is $0.13 \%$.
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# Model independent search for new phenomena in $p \bar{p}$ collisions at $\sqrt{s}=1.96 \mathrm{TeV}$ 

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We describe a model-independent search for physics beyond the standard model in lepton final states. We examine 117 final states using $1.1 \mathrm{fb}^{-1}$ of $p \bar{p}$ collisions data at $\sqrt{s}=1.96 \mathrm{TeV}$ collected with the D 0 detector. We conclude that all observed discrepancies between data and model can be attributed to uncertainties in the standard model background modeling, and hence we do not see any evidence for physics beyond the standard model.

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## I. INTRODUCTION

The standard model (SM) has been remarkably successful in accommodating all the interactions between the fundamental particles [1]. Despite this success, there are strong motivations to expect new phenomena at energies at the order of the electroweak scale. For example, the Higgs boson [2] receives quantum corrections to its mass through loop diagrams. The scalar nature of the Higgs boson leads to a quadratic divergence, with an upper limit of the integral set by the highest scale, i.e., the Planck mass $\left(10^{19} \mathrm{GeV}\right)$. To maintain the Higgs mass close to the

[^78]electroweak scale, it is necessary to fine-tune a parameter in the theory to within $M_{W} / M_{\text {Planck }} \approx 10^{-16}$ [3].

There are few logical options for overcoming this problem. If the Higgs boson does not exist, then there must be a new contribution to the physics at the electroweak scale. If the Higgs boson does exist, then the theory must be either fine-tuned or a generalized Higgs scheme, beyond the SM, is present at the electroweak scale.

Assuming that beyond standard model physics exists, we do not know how it appears, rendering its search difficult. While there are many theories that predict observable differences with the SM, these models usually depend on additional unspecified parameters which broaden the possible range of results.

Motivated by uncertainty and expectations of physics beyond the SM, we examine data from many channels in $p \bar{p}$ collisions at $\sqrt{s}=1.96 \mathrm{TeV}$ at the Tevatron Collider at Fermilab, collected by the D0 experiment, for deviations from the SM. After this, we focus on events with objects with high transverse momentum $\left(p_{T}\right)$ in a quasi-modelindependent search for new phenomena effects. Similar approaches have been applied to data from the D0

Collaboration [4-6], the H1 Collaboration at the HERA ep collider at DESY [7], and the CDF Collaboration at the Tevatron [8,9].

Our technique trades the sensitivity of specific searches for breadth of coverage: we do not design selections focused on a particular model and neglect systematic uncertainties. This way, we can incorporate many channels without developing a detailed modeling for each individual channel. This approach limits sensitivity for physics beyond the SM in individual final states, but it helps identify global differences relative to the SM expectations. If any particular final state or distribution found discrepant with the SM remains significantly discrepant after systematic uncertainties are considered, then it warrants claim for the presence of physics beyond the SM. The benefit of this approach is that we can look in a coordinated way at many channels, applying expectations from the SM and a model of the detector in a relatively straightforward manner, to search for discrepancies between data and the SM.

The data for this search consists of events containing high $p_{T}$ objects. The SM background estimates are based on Monte Carlo (MC) predictions supplemented with datadriven estimates of backgrounds where a jet fakes a lepton (multijet backgrounds). We apply corrections to the MC simulation, determined either from previous D0 studies based on well-understood regions of phase space or from higher-order MC simulations. These corrections are discussed further in Sec. IV.

We divide the data and the selected MC simulated events into seven inclusive subsets based on the number and types of leptons identified in each event. Unlike the search conducted by the CDF Collaboration [8,9], only events with at least one electron or muon are considered. To account for any incorrect normalizations in the absence of higher-order corrections to the cross section calculations, and for experimental systematic uncertainties, we determine scale factors for the MC contributions by fitting kinematic distributions in each of the seven inclusive subsets, as discussed in Sec. V.

The seven nonoverlapping inclusive subsets are merged to provide input for the analyses employing algorithms called VISTA and SLEUTH [8], as discussed in Sec. VII. In brief, VISTA searches for deviations in bulk distributions, while SLEUTH looks for excesses of data in the high- $p_{T}$ tails.

## II. D0 DETECTOR

The data correspond to $1.07 \pm 0.07 \mathrm{fb}^{-1}$ of integrated luminosity from $p \bar{p}$ collisions at the Tevatron Collider at Fermilab, collected with the D0 detector at $\sqrt{s}=$ 1.96 TeV during 2002-2006.

The D0 detector is described in detail elsewhere [10]. The central tracking, calorimetry, and muon systems are the components most important to this analysis. The central tracking system consists of a silicon microstrip tracker (SMT) and a central fiber tracker, both located within a 2 T
superconducting solenoidal magnet, and provides charged particle tracking for pseudorapidities $|\eta|<3$, where $\eta=$ $-\ln [\tan (\theta / 2)]$, and $\theta$ is the polar angle relative to the center of the detector with respect to the proton beam direction.

The three liquid-argon/uranium calorimeters are housed in separate cryostats. Outside of the tracking system, a central section covers up to $|\eta|=1.1$. Two end calorimeters extend coverage to $|\eta|=4.2$. The calorimeter is highly segmented with four electromagnetic (EM) and four to five hadronic longitudinal layers; transverse to the particle direction, typical segmentation is $\Delta \eta=\Delta \phi=$ 0.1 , where $\phi$ is the azimuthal angle.

Beyond the calorimeter, a muon system consists of a layer of tracking detectors and scintillation trigger counters in front of 1.8 T iron toroids, followed by two similar layers after the toroids, all at pseudorapidities $|\eta|<2.0$ [11].

A three-level trigger system selects events, recording data at about 100 Hz . Our sample was collected using triggers that select events with at least one electron or one muon. The same trigger requirements are applied in the selection of the data samples used for the estimation of the multijet backgrounds.

## III. OBJECT ID AND EVENT SELECTION

In this section, we describe the identification criteria used to select energetic objects isolated from other event activity, viz., electrons ( $e^{ \pm}$), muons ( $\mu^{ \pm}$), tau leptons ( $\tau^{ \pm}$), missing transverse energy $\left(\mathscr{E}_{T}\right)$, jets, and $b$-quark jets. In addition, we discuss the criteria used to select samples of nonisolated electrons and muons. These objects are used to estimate the contribution of instrumental backgrounds to our final states. Objects that pass very loose isolation criteria but fail the tighter isolation criteria used for our signal events are primarily from jets. Events with these objects passing very loose isolation criteria are kinematically similar to events where the jet successfully mimics an isolated lepton. The number of these events in each final state is determined as part of the inclusive normalization fits, detailed in Sec. VI.

## A. Vertices

Only $p \bar{p}$ interaction vertices reconstructed from at least three tracks are allowed in this analysis. Based on the $p_{T}$ of the tracks associated with that vertex, we define the primary $p \bar{p}$ interaction vertex (PV), as the one with smallest probability of originating from a minimum-bias interaction [12]. The $z$ coordinate of the $\mathrm{PV}\left(z_{\mathrm{PV}}\right)$ is required to be $\left|z_{\mathrm{PV}}\right|<$ 60 cm (where the positive $z$ axis is oriented along the proton beam direction, with origin at the center of the detector).

## B. Electrons

Electrons are characterized by an isolated shower in the calorimeter and an isolated track in the central tracker.

Starting with a seed cell, a calorimeter cluster is formed using cells within a cone of radius $\Delta \mathcal{R}<0.4$ where $\Delta \mathcal{R}=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}$. Such clusters are required to pass the calorimeter isolation criterion $\left(E_{\text {tot }}(\Delta \mathcal{R}<0.4)-\right.$ $\left.E_{\mathrm{EM}}(\Delta \mathcal{R}<0.2)\right) / E_{\mathrm{EM}}(\Delta \mathcal{R}<0.2)<0.2$, where $E_{\mathrm{tot}}$ is the total energy of the shower, summing the EM and hadronic calorimeter cells, and $E_{\text {Ем }}$ is the energy in the EM calorimeter only. Every accepted cluster must have $90 \%$ of $E_{\text {tot }}$ within the EM calorimeter, pass a $\chi^{2}$-based selection on the spatial distribution of the shower, and be matched with a track extrapolated from the central tracker. An electron likelihood ( $L_{e}$ ), based on seven tracking and calorimetric parameters, is used to enhance signal purity of the candidate electrons. Different selection criteria on $L_{e}$ are used for different final states, as discussed in Sec. V.

In this analysis, we use only electrons that are found in the central calorimeter, with $|\eta|<1.1$ and $p_{T}>15 \mathrm{GeV}$. Typical electron detection efficiencies are $70 \%$ to $80 \%$.

To estimate the contribution from nonisolated electrons (e.g., from multijet background), we use the same selection as for signal, but with a reversed $L_{e}$ likelihood criterion.

## C. Muons

Muons are identified in the muon system, and then matched to tracks. They are required to have $|\eta|<1.5$ and $p_{T}>15 \mathrm{GeV}$. The track requirements include a selection on DCA $<0.02$ ( 0.2 ) cm for tracks with (without) hits in the SMT, where DCA is the distance of closest approach of the track to the PV in the transverse plane.

We require muons to be isolated, meaning that the sum of the transverse energies in calorimeter cells in an annular region $(0.1<\Delta \mathcal{R}<0.4)$ around the muon track, and the sum of the tracks $p_{T}$ in a cone of $\Delta \mathcal{R}<0.5$ around the muon track must both be less than 2.5 GeV .

To estimate the multijet background in the single muon sample, we use control samples where the isolation variables are required to be between 2.5 GeV and 8 GeV . All other criteria are the same as in the signal data sample.

Because the muon $p_{T}$ is estimated by the $p_{T}$ of the matching track in the central tracker, the momentum resolution decreases with increasing $p_{T}$. To restrict the analysis to muons with well measured momenta, we require the significance of its $p_{T}$ measurement to be $\left(1 / p_{T}\right) / \sigma\left(1 / p_{T}\right)>3$, where $\sigma\left(1 / p_{T}\right)$ is the uncertainty on the measurement of the track curvature (inverse of the muon track's $p_{T}$ ). This effectively limits muons to $p_{T}<200 \mathrm{GeV}$.

## D. Tau leptons

Tau leptons can decay to $e \nu_{e} \nu_{\tau}, \mu \nu_{\mu} \nu_{\tau}$, or hadrons $h \nu_{\tau}$ $\left(\tau_{h}\right)$. It is difficult to determine whether a light lepton in an event originated from a $\tau$, but the signature from $\tau_{h} \rightarrow h \nu_{\tau}$ differs significantly from that of a jet. The decays $\tau \rightarrow \pi \nu_{\tau}$ are referred to as Type-1. Decays corresponding to $\tau^{ \pm} \rightarrow$ $\pi^{ \pm} n \pi^{0} \nu_{\tau}$ are referred to as Type-2 ( $n$ is an integer $\geq 1$ ),
and decays to multiple charged pions are referred to as Type-3 decays. Type-3 decays differ from Type-1 ( $\tau_{1}$ ) and Type-2 $\left(\tau_{2}\right)$ by being matched to multiple tracks, and are not used in this analysis. Type-1 and Type-2 decays are required to have $|\eta|<1.1$ and a track with at least one SMT hit, as well as $p_{T}>10 \mathrm{GeV}$ for Type-1, and $p_{T}>$ 5 GeV for Type-2 tau leptons. There are also requirements concerning overlaps of objects: $\Delta \mathcal{R}(\mu, \tau)>0.4$ and $\Delta \mathcal{R}(e, \tau)>0.4$, where $\tau, \mu$ and $e$ are as defined above, except that muons that pass the overlap criterion do not have to pass the additional isolation requirement. To distinguish $\tau_{h}$ decays from jets, we use a neural network discriminant [13], $\mathrm{NN}_{h}$, and to distinguish Type-2 $\tau_{h}$ from electrons, we use an additional neural network, $\mathrm{NN}_{e}$. We require $\mathrm{NN}_{h}>0.9$ for $\tau_{1}$ and $\tau_{2}$, and $\mathrm{NN}_{e}>0.2$ for $\tau_{2}$.

To model the multijet contribution to final states with $\tau_{h}$ decays, we select events with $\tau_{h}$ candidates as above, but with $0.3<\mathrm{NN}_{h}<0.8$.

## E. Jets

We reconstruct jets within $|\eta|<2.5$, using an iterative midpoint cone algorithm [14] with cone radius of 0.5 and a minimum $p_{T}$ requirement of 20 GeV after applying a jet energy scale (JES) correction as discussed in Sec. IV B 3. Jets separated from a $\tau_{h}$ or an electron by $\Delta \mathcal{R}<0.5$ are removed from consideration.

## F. $b$-jets

Bottom and charm quarks can travel measurable distances from the PV before decaying, so that their decay products originate from an identifiable secondary vertex. This provides a way of tagging jets coming from a $b(c)$-quark decay by examining the associated tracks [15]. Before applying any $b$-tagging criteria, the jets are required to pass both calorimeter criteria outlined in Sec. IIIE and the taggability criteria. A jet is taggable if it is matched to a track jet, which is a jet formed from tracks, reconstructed using a simple cone-clustering algorithm of $\Delta \mathcal{R}<0.5$. At least two tracks are required, with at least one having $p_{T}>1 \mathrm{GeV}$ and another with $p_{T}>0.5 \mathrm{GeV}$. Every track in the jet is required to have at least one hit in the SMT detector, a DCA $<0.2 \mathrm{~cm}$, and a distance of closest approach along the $z$ axis of $<0.4 \mathrm{~cm}$.

All taggable jets are subjected to a neural network $b$ tagging algorithm [15] whose input variables include the DCA of each track in a jet and information on secondary vertices in the jet. We define $b$-jet candidates by requiring that the neural network output be greater than 0.775 . This algorithm selects about $60 \%$ of $b$ jets with $p_{T}=50 \mathrm{GeV}$, and only $1 \%$ of light flavor ( $u, d, s$ quarks or gluon) jets.

## G. Missing transverse energy

Neutrinos or other weakly-interacting neutral particles do not leave energy deposits in the detector. Their presence
is inferred from the measurement of significant $\mathbb{E}_{T}$ in the event. The missing transverse energy is determined from energies deposited in all calorimeter cells. The $\mathscr{E}_{T}$ is corrected for JES, measured muon $p_{T}$, electron and $\tau_{h}$ energy scales. The JES-corrected $\mathbb{E}_{T}$ vector is obtained by adding the difference between the vector sums of uncorrected and JES-corrected jet momenta to the uncorrected $\mathscr{E}_{T}$ vector. The muon correction reflects the fact that muons deposit little energy in the calorimeter, and adjusts the $\mathbb{E}_{T}$ for the $p_{T}$ of the muon. Finally, electron and $\tau_{h}$ energy corrections are applied to the appropriate calorimeter cells in the $\mathscr{E}_{T}$ calculation.

## IV. MODELING SM PREDICTIONS

## A. SM event generation

We generally estimate SM processes with MC-generated events. A model-independent search incorporates many different processes to properly model the data. We use two generators for this purpose, ALPGEN [16] for generation of all processes, except for diboson production which is generated with PYTHIA [17]. PYTHIA is also used for hadronization and showering.

ALPGEN uses exact matrix elements at leading orders for QCD and electroweak interactions. The benefit of using ALPGEN comes from its ability to calculate exact leadingorder terms for processes that include high jet multiplicities. ALPGEN produces parton-level events with information on color and flavor, and can be matched to PYTHIA for parton evolution and hadronization.

Matching of a parton from ALPGEN to PYTHIA showering has the fundamental difficulty of separation of the hard interaction from initial-state radiation and final-state radiation. To address this problem we use the MLM matching scheme [18]. In this scheme each final-state parton from the matrix element is matched in $\Delta \mathcal{R}$ to an evolved jet. We further reject events which contain an additional jet not matched to a final-state parton, except in the sample with the highest number of final-state partons.

The following processes are considered, where $j$ is a light jet ( $g, u, d$, or $s$ ), $\ell$ is a lepton, $N$ is an integer $\geq 0$ and $l p$ represents a light parton:
(1) $W+N j$,
(2) $Z / \gamma^{*}+N j$,
(3) $W+c \bar{c}+N j$,
(4) $W+b \bar{b}+N j$,
(5) $Z / \gamma^{*}+c \bar{c}+N j$,
(6) $Z / \gamma^{*}+b \bar{b}+N j$,
(7) $t \bar{t} \rightarrow(2 \ell+2 \nu+2 b)+N j$,
(8) $t \bar{t} \rightarrow(\ell \nu+2 b+2 l p)+N j$,
(9) $W W$,
(10) $W Z$,
(11) $Z Z$.

Since this analysis does not include events with identified photons, we do not consider the contributions to the
background from the $W \gamma$ and $Z \gamma$ processes. The processes involving heavy flavor (HF) quarks ( $c$ and $b$ ) are treated separately from light quark processes because they are often associated with particularly interesting final states, and we generate large number of MC events for these final states. Some of these processes are included in the lightparton simulations, so we remove the events with heavy flavor quarks from the light-parton samples so as to avoid double-counting.

For some objects, other programs provide more accurate simulations of their properties and decays. Specifically, TAUOLA [19] is used for $\tau$ decays, and EVTGEN [20] is used for the decay of $b$ hadrons. Where needed, correction factors for the cross sections, corresponding to contributions from higher-order diagrams, are determined through the normalization procedure based on the inclusive final states as discussed in Sec. V.

We assume a mass of 172.5 GeV for the top quark, consistent with recent measurements [21].

## B. Detector simulation

The events produced from the above combination of generators are processed through the D0 detector simulation and combined with random beam crossing events taken from data (Sec. IV B 1). The detector simulation is based on GEANT 3.2.1[22], to which two types of correction factors are applied. The first type of correction is event reweighting, where an overall correction is applied to the MC event, rather than to the measured kinematic properties of reconstructed objects. For example, we apply weights to account for the difference in reconstruction efficiencies between data and MC. Another type of correction modifies the objects in a MC event to account for the fact that the simulation has better resolution and a different energy scale than the detector. These corrections generally depend on properties of the objects in an event. The specific corrections used in this analysis are described below.

## 1. Instantaneous luminosity reweighting

As the instantaneous luminosity profiles of the random beam crossing events and the data are not identical, the MC is reweighted to match the instantaneous luminosity distribution in data. During the course of the data-taking period corresponding to the data used for this search the number of average collisions per beam crossing increased from two to six.

## 2. $Z_{\mathrm{PV}}$ Reweighting

Our simulated events have a narrower $z_{\mathrm{PV}}$ distribution than is observed in data. We therefore apply a weight to each event, based on the $z_{\mathrm{PV}}$ of the event, to increase the relative weight of events farther from the center of our detector to match the observed distribution.

## 3. JES

We apply JES corrections to jets in both data and MC [23]. The purpose of the JES corrections is to correct the measured jet energy to that of the particles in the jet. Jet energies initially determined from the calorimeter cell energies do not exactly correspond to the energies of final-state particles that traverse the calorimeter. As a result, a detailed calibration is applied separately in data and MC. In general, the energy of all final-state particles inside the jet cone, $E_{j}^{\mathrm{ptcl}}$, can be related to the energy measured inside the jet cone, $E_{j}$, by $E_{j}^{\mathrm{ptcl}}=\left(E_{j}-O\right) /(R S)$. Here, $O$ denotes an offset energy, primarily from additional interactions in or out of time with an event. $R$ is the average response of the calorimeter to the particles in a jet, and $S$ is the correction factor for the net energy loss from particles that scatter out of or into the jet cone. For a given cone radius, $O$ and $S$ are functions of the jet $\eta$ within the detector. $O$ is also a function of the number of reconstructed event vertices and the instantaneous luminosity; $R$ is the largest correction factor and reflects the lower response of the calorimeter to charged hadrons relative to electrons and photons. It also includes the effect of particle energy loss in front of the calorimeter. The primary response correction is derived from studies of $\gamma+$ jet events, and depends on jet energy and pseudorapidity. For all jets that contain nonisolated muons, we add the muon momenta to that of the jet. Under the assumption that these muons are from semileptonic decays of $b$ quarks, we also add an estimated average neutrino momentum assumed to be collinear with the jet direction.

## 4. Jet shifting, smearing, and removal

Additional corrections beyond the JES are needed to take into account threshold and resolution effects for jets. The jet shifting, smearing, and removal corrections are determined from $Z / \gamma \rightarrow e e+1$ jet events. The $Z / \gamma$ and the jet should be produced approximately back-to-back in $\phi$ with the same $p_{T}$. This is quantified by a $p_{T}$ imbalance variable, $\Delta S=\left(p_{T}^{j}-p_{T}^{Z / \gamma}\right) / p_{T}^{Z / \gamma}$. For jets with a $p_{T}$ well above the reconstruction threshold, the distribution of $\Delta S$ is Gaussian in both data and MC. The difference in the means of these distributions yields a shift that is applied to the MC jet energies to match the data, and a smearing is applied to MC jets based on the difference in the standard deviations of these distributions. Jets that fail the $p_{T}>$ 20 GeV requirement after shifting and smearing corrections are removed from further consideration.

## 5. Efficiencies

The efficiency of the MC simulation of our detector tends to be larger than the true efficiency of the detector. To account for this, we introduce scale factors to adjust the MC efficiency to match that observed in data. The efficiencies for electrons and muons are obtained using $Z \rightarrow$
$e e$ and $Z \rightarrow \mu \mu$ events. One of the decay products of the $Z$ boson is the tag object, which is required to pass restrictive reconstruction requirements and be matched to an object that could have fired the trigger for the event. Object efficiencies are then obtained using the second object from the $Z$ decay.

## 6. Track $P_{T}$ resolution

Electron energies are measured in the calorimeter. However, energy deposition does not depend on the charge of the electron, which is determined by the curvature of the associated track in the magnetic field. An incorrectly reconstructed track can therefore lead to an incorrect charge assignment. Bremsstrahlung from electrons can affect the curvature of the tracks. Also, a soft interaction in the inner detector can result in the process $e^{+} \rightarrow e^{+} e^{-} e^{+}$, leading to charge misidentification if the wrong sign electron track is associated with the electron. This difficulty is also present in tau decays when at least one hadron is produced.

Because the rate of charge misidentification is not properly modeled in the detector simulation, we add a scale factor to electron and tau MC events to approximate the appropriate rate of charge misidentification. We determine this scale factor by using dielectron events consistent with $Z \rightarrow e e$ decays; and we only consider events with dielectron invariant mass between 70 to 110 GeV to avoid biases against physics beyond the SM. The charge misidentification rate in data is about $1 \%$, while the MC predicts a rate of $0.5 \%$.

The disagreement in track resolution between the data and MC also affects muon $p_{T}$ measurement, which is corrected using smearing parameters determined by comparing the data and MC mass peaks for $Z \rightarrow \mu \mu$ and $J / \psi \rightarrow \mu \mu$ decays.

## 7. Electron energy smearing

In the simulation, the electron $p_{T}$ reconstructed in the calorimeter has a better resolution than in the data. We correct this using a Gaussian smearing function tuned to reproduce the shape of the $Z \rightarrow e e$ peak.

## 8. Jet taggability

The jet taggability rates (Sec. IIIF) are found to be different for MC and data. To correct for this difference, correction factors are applied as scale factors depending on $p_{T}, \eta$ and $z_{\mathrm{PV}}$ of the jet [24].

## 9. b-tagging rate

As detailed in Sec. III F, we apply a tagging algorithm to both data and MC jets to select jets originating from heavy $(b / c)$ quarks. However, the algorithm can select mistagged light jets. The tagging rates (for both heavy- and lightparton jets) depend on the $p_{T}$ and $\eta$ of the jets. The heavyquark tagging rates are measured separately in both data
and MC using dedicated samples. The performance of the $b$-tagging algorithm in MC events is better than in data. To correct the tagging rates in MC events, we first determine the flavor of the tagged jet by matching it in $\Delta \mathcal{R}$ with the initial parton. Depending on the flavor of the jet, we apply a per-jet scale factor given by $\mathrm{SF}=\epsilon^{\mathrm{data}}\left(p_{T}, \eta\right) / \epsilon^{\mathrm{MC}}\left(p_{T}, \eta\right)$, where $\epsilon^{\text {data }}\left(p_{T}, \eta\right)$ and $\epsilon^{\mathrm{MC}}\left(p_{T}, \eta\right)$ are the $b$-tagging efficiencies for a given parton flavor for data (MC) events. To maintain correct normalization, a small downward correction is applied to non- $b$-tagged jets.

## 10. Weak gauge boson $p_{T}$

The $p_{T}$ distribution of the $Z$ boson from alpgen MC is corrected to match the distribution observed in data in $Z \rightarrow e e$ decays [25]. A modified reweighting is carried over to the $W$ boson $p_{T}$ based on the theoretical ratio of the $W$ to $Z p_{T}$ spectra [26].

## 11. $\Delta \phi$

We apply a $\Delta \phi$-dependent weight derived specifically for this analysis using the inclusive distributions described in Sec. V to correct the $\Delta \phi$ between leptons in dilepton final states and the lepton and $\mathbb{E}_{T}$ in single-lepton + jets final states. This additional correction is required because the limited detector resolution at small $p_{T}$ values prevents us from obtaining a good description of the $\Delta \phi$ distribution in the region $p_{T} \approx 0$, which is dominated by SM processes, by using only the correction on the weak boson

TABLE I. Inclusive final states and their object selections, where $p_{T}^{\min }$ is the minimum allowed value of $p_{T}$ and $|\eta|^{\max }$ is the maximum allowed value of $|\eta|$.

| Final state | Object | $p_{T}^{\min }(\mathrm{GeV})$ | $\|\eta\|^{\max }$ |
| :---: | :---: | :---: | :---: |
| $e+$ jets $+X^{\mathrm{a}}$ | $e$ | 35 | 1.1 |
|  | jet | 20 | 2.5 |
|  | $\not E_{T}$ | 20 | - |
| $\mu+$ jets $+X^{\mathrm{b}}$ | $\mu$ | 25 | 1.5 |
|  | jet | 20 | 2.5 |
| $e e+X^{\mathrm{c}}$ | $\not$ T $_{T}$ | 20 | - |
| $\mu \mu+X^{\mathrm{d}}$ | $e$ | 20 | 1.1 |
| $\mu e+X^{\mathrm{e}}$ | $\mu$ | 15 | 1.5 |
|  | $\mu$ | 15 | 1.5 |
| $e \tau+X^{\mathrm{f}}$ | $e$ | 15 | 1.1 |
|  | $e$ | 15 | 1.1 |
| $\mu \tau+X^{\mathrm{g}}$ | $\tau$ | 15 | 1.1 |
|  | $\mu$ | 15 | 1.5 |

${ }^{\mathrm{a}} X \neq e, \mu, \tau, \gamma$
${ }^{\mathrm{b}} X \neq e, \mu, \tau, \gamma$
${ }^{\mathrm{c}} X \neq \mu, \tau, \gamma$
${ }^{\mathrm{d}} X \neq e, \tau, \gamma$
${ }^{\mathrm{e}} X \neq \tau, \gamma$
${ }^{\mathrm{t}} X \neq \gamma$
${ }^{\mathrm{g}} X \neq e, \gamma$
$p_{T}$ [27]. We remove events containing high $p_{T}$ objects, using the same method described in Sec. VI, from the fit to avoid introducing biases from possible new physics signals. This reweighting affects not only the $\Delta \phi$ distributions, but also other quantities that depend on the angular distribution of particles such as the $p_{T}$ of the $W$ boson.

## V. INCLUSIVE FINAL STATES

To determine the unknown scale factors from the data, we construct seven inclusive final states each dominated by a specific SM process. These seven inclusive nonoverlapping final states are specified in Table I by the relevant objects and their selection criteria. The additional objects ( $X$ in the table) are selected as shown in Table II. We reject events that include a photon in the central calorimeter with a $p_{T}>15 \mathrm{GeV}$, mainly due to difficulties in modeling. Events with real photon misidentified as electrons could contaminate the $e+$ jets, and the dilepton or trilepton final states containing at least one electrons. We have estimated the contributions from such backgrounds and consider them negligible in the region of the phase space that is relevant for the search for physics beyond the SM. The seven states $(e+$ jets, $\mu+$ jets, $e e, \mu \mu, \mu e, e \tau, \mu \tau)$ were each selected to correspond to a specific SM process.
(i) $e+$ jets

The electron + jets final states have more background from multijet events, where a jet is misidentified as an electron, than the other electron final states. Therefore the likelihood criterion used is tighter than in other final states, $\mathcal{L}_{e}>0.95$. We also require at least one jet having $E_{T}>20 \mathrm{GeV}$, $\mathbb{E}_{T}>20 \mathrm{GeV}$, and an $e p_{T}>35 \mathrm{GeV}$. This final state is dominated by $W+$ jets events with $W \rightarrow$ $e \nu$ decays. The multijet background in this final state is estimated using a sample of events with exactly one nonisolated electron with a $p_{T}>35 \mathrm{GeV}$ and the same jet and $\mathbb{E}_{T}$ criteria as in signal.
(ii) $\mu+$ jets

The $\mu+$ jets final state is dominated by $W+$ jets events with $W \rightarrow \mu \nu$ decays. To reduce the amount of multijet background, at least one jet having $E_{T}>$ 20 GeV is required, as well as $\mathscr{E}_{T}>20 \mathrm{GeV}$ and a muon with $p_{T}>25 \mathrm{GeV}$. Just as with the $e+$ jets final state, this final state is inclusive in jets with

TABLE II. Criteria required for inclusion as additional objects $(X)$ in one of the seven final states listed in Table I.

| Object | $p_{T}^{\min }(\mathrm{GeV})$ | $\|\eta\|^{\max }$ |
| :---: | :---: | :---: |
| $e$ | 15 | 1.1 |
| $\mu$ | 15 | 1.5 |
| $\tau$ | 15 | 1.1 |
| jet | 20 | 2.5 |

no other additional objects allowed. The multijet background in this final state is estimated using a sample of nonisolated muons with $p_{T}>25 \mathrm{GeV}$ and the same jet and $\mathscr{H}_{T}$ requirements as isolated muons.
(iii) $e e$

The dielectron final state requires each electron to have $p_{T}>20 \mathrm{GeV}$ and $\mathcal{L}_{e}>0.85$. The electrons are also restricted to be in the central calorimeter, $|\eta|<1.1$, and the jets have the same criteria as for the other final states. This final state is dominated by $Z / \gamma^{*} \rightarrow e e$ events. No multijet background is necessary in this channel to produce a satisfactory normalization fit.
(iv) $\mu \mu$

The dimuon final state requires at least two muons with the muon- $p_{T}$ criteria lowered to $p_{T}>15 \mathrm{GeV}$ because of the smaller contribution from multijet background. Any jet must have $p_{T}>20 \mathrm{GeV}$. This final state is inclusive in both jets and muons, but an additional $e$ or $\tau$ lepton places the event in the $\mu e$ or $\mu \tau$ final states. Analogous to the $e e$ channel, this final state is dominated by $Z / \gamma^{*} \rightarrow \mu \mu$ events. No multijet background is necessary in this channel to produce a satisfactory normalization fit.
(v) $\mu e$

The $\mu$ e final state is inclusive except for $\tau$ leptons; $e \mu \tau$ events are assigned to the $e \tau$ final state. This final state is dominated by $Z / \gamma^{*} \rightarrow \tau \tau$ events. The multijet background in this final state is estimated from a sample consisting of nonisolated electrons and isolated muons, and contains both multijet and $W+$ jet events.
(vi) e $\tau$

The $e \tau$ sample is inclusive in all objects. The electron and $\tau_{h} p_{T}$ are required to be at least 15 GeV . The electron likelihood is set to $L_{e}>$ 0.95 to reduce the large multijet background as many apparent $\tau_{h}$ correspond to misidentified jets. The parameter that separates electron from hadronic taus, $\mathrm{NN}_{e}$, is set to 0.8 to reduce the contribution from dielectron events. This final state is also dominated by $Z / \gamma^{*} \rightarrow \tau \tau$ events. The multijet background in this final state is estimated from a sample of isolated electrons and nonisolated $\tau$ leptons, and contains both multijet and $W+$ jet events.

The $\mu \tau$ state contains at least one muon and one $\tau_{h}$. It is inclusive in all objects except electrons, whose presence would move the event to the $e \tau$ final state. This final state is also dominated by $Z / \gamma^{*} \rightarrow \tau \tau$ events. The multijet background in this final state is estimated from a sample of isolated muons and nonisolated $\tau$ leptons, and contains both multijet and $W+$ jet events.

## VI. INCLUSIVE NORMALIZATION FITS

Our model does not provide proper normalization of different MC contributions because, for example, of higher-order corrections needed for the leading-order or leading-logarithm cross section calculations. To avoid uncertainties in normalization, we perform a fit, described below, for each of the inclusive final states to obtain scale factors that reproduce the distributions of the selected data using a combination of the SM MC and multijet predictions determined from data. We treat the Drell-Yan (D-Y) contributions to the $e e$ and $\mu \mu$ final states without light partons separately from those with light partons because it improves agreement between data and MC.

The fits for normalization factors are performed on kinematic distributions of different object quantities, altering the overall normalization of each input process contributing to the final state so that the $\chi^{2}$ probability for that final state is minimized for the combined fit. To avoid fitting to data at the highest values of $p_{T}$, where new physical processes can be important, we only use events that are not in the high $p_{T}$ tail, which is defined as containing $10 \%$ of the events. Distributions of basic quantities such as $\mathscr{L}_{T}, p_{T}, \eta, \Delta \phi\left(\mathrm{obj}, \mathscr{C}_{T}\right)$ of leptons and jets (here obj refers to the momentum vector of the object considered) are used in the fits while more complex variables are used to check the quality of the overall fit. The latter variables include the mass or transverse mass $M_{T}=$ $\sqrt{\left(p_{T, 1}+p_{T, 2}\right)^{2}-\left(\vec{p}_{T, 1}+\vec{p}_{T, 2}\right)^{2}}$ of two or more objects, jet multiplicities, and the $p_{T}$ of the $W$ and $Z$ bosons. If an event contains any object outside the $p_{T}$ range defined above, then none of the objects in the event are used in the fit.

The list of the seven final states, the processes that are normalized through the inclusive fits to each of the final states, and the number of events in each final state are shown in Table III. Once the fitted values are extracted, the distributions are rescaled accordingly, and the total background contribution, $B$, for a particular final state is

$$
\begin{equation*}
B=\sum_{i}^{N_{\text {bkg }}} S_{i} B_{i} \tag{1}
\end{equation*}
$$

where the scale factor $\left(S_{i}\right)$ for each background process $\left(B_{i}\right)$ is determined from the final state in which its contribution is most important and that scale factor is used in all other final states to which that background contributes. $N_{\text {bkg }}$ refers the total number of all the SM processes contributing to a particular final state.

A simplified example for the $e+$ jets $+X$ final state ( $X \neq e, \mu, \tau, \gamma$ ) is used to illustrate the procedure. The $e+$ jets $+X$ state is dominated by $W \rightarrow e \nu$ events, but there is a significant contribution from multijet and DrellYan events. We use the normalization factor for the Drell-

TABLE III. The contributions used in the inclusive fits for each of the inclusive final states and the number of selected data events in each. The dominant SM process is listed first for each final state. In the $e \tau$ and $\mu \tau$ final states, the multijet background also includes a contribution from $W+$ jets.

| State | SM process | Events |
| :---: | :---: | :---: |
| $e+$ jets $+X$ | $W+$ jets | 40 k |
|  | Multijet |  |
|  | $W / Z+\mathrm{HF}$ | 50 k |
|  | $W+$ jets $+X$ | Multijet |
|  | $W / Z+\mathrm{HF}$ |  |
|  | D-Y $+0 l p$ |  |
|  | D-Y1 $-3 l p$ | 25 k |
|  | $W / Z+\mathrm{HF}$ |  |
| $\mu \mu+X$ | $\mathrm{D}-\mathrm{Y}+0 l p$ | 24 k |
|  | $\mathrm{D}-\mathrm{Y}+1-3 l p$ |  |
|  | $W / Z+\mathrm{HF}$ |  |
| $\mu e+X$ | $Z \rightarrow \tau \tau$ | 0.34 k |
|  | Multijet | 1.3 k |
| $e \tau+X$ | $Z \rightarrow \tau \tau$ |  |
|  | Multijet |  |
|  | $Z \rightarrow e e$ | 1.0 k |
| $\mu \tau+X$ | $Z \rightarrow \tau \tau$ |  |

Yan process, determined through a separate fit to the $e e+$ $X$ final state $(X \neq \mu, \tau, \gamma)$, in the $e+$ jets fit. We also fix the scale factors to one for rare processes which have contributions that are too small to fit accurately in $e+$ jets, such as the $t \bar{t}$ contribution. We then fit for the SM $W$ boson and multijet contributions in the data. The fit optimizes agreement between the distributions in data and the SM prediction for the variables listed above. The result of the fit is two overall weights, one for $W \rightarrow e \nu$ and one for multijet $\rightarrow e+$ jets.

In the $e e$ and $\mu \mu$ final states, there are three contributions allowed to float relative to each other, $Z+0 l p, Z+$ $1-3 l p$, and the number of $W / Z+$ hf events. In the $e+$ jets and $\mu+$ jets, the $Z$ contribution is held fixed to the values found in the $e e$ and $\mu \mu$ fits, and the $W+l p$, multijet, and $W+\mathrm{hf}$ contributions are allowed to float. In the $\mu \tau$, and $\mu e$ final states, the multijet and $Z \rightarrow \tau \tau$ contributions are allowed to float, while other $Z$ contributions are fixed to values given by the fits to the $e e$ and $\mu \mu$ final states. The $e \tau$ final state is similar, but the $Z \rightarrow e e$ contribution is large enough that we also allow the normalization of this contribution to float. In all final states, the number of $t \bar{t}$ and diboson events are held fixed to the best available calculations of the cross sections (approximate next-to-next-to-leading-order for $t \bar{t}$ and next-to-leading-order for $W W$ ) [28]. The ratio of $W / Z+b \bar{b}$ to $W / Z+c \bar{c}$ are also held fixed to the expected ratio from next-to-leading-order calculations [29].



FIG. 1 (color online). $\quad e+$ jets final state (a) electron $p_{T}$ histogram and (b) transverse mass ( $e, \mathbb{E}_{T}$ ) check histogram.

The distributions of the variables for the input processes are not varied, only their relative contributions. The fit is performed using the MINUIT program [30]. For singlelepton states and hadronic $\tau$ final states, multijet events are a significant background. We assume that the contribution from other SM processes modeled by the MC samples to the multijet background is small. The scale


FIG. 2 (color online). $\quad \mu+$ jets final state (a) $\mathscr{E}_{T}$ histogram and (b) transverse mass $\left(\mu, \mathscr{E}_{T}\right)$ check histogram.


FIG. 3 (color online). ee final state (a) leading electron (with highest $\left.p_{T}\right) p_{T}$ fit histogram and (b) invariant mass $(e, e)$ check histogram.
factors of input processes for the MC events should also account for the contributions of the processes to the multijet background. The main effects of contributions from any of the MC processes to the multijet background would be to decrease the scale factor for backgrounds modeled by MC.


FIG. 4 (color online). $\quad \mu \mu$ final state (a) leading muon $p_{T}$ fit histogram and (b) invariant mass ( $\mu, \mu$ ) check histogram.


FIG. 5 (color online). $\mu e$ final state (a) electron $p_{T}$ fit histogram and (b) invariant mass ( $\mu, e$ ) check histogram.

The main purpose of the normalization process is to assure that the fundamental SM processes are wellmodeled. The results of the fit are then checked for qualitative agreement with the data. The overall scale factors are checked to compare to those from dedicated analyses. If the normalization factors are properly included in the MC , then all the scale factors should equal unity. In the $e+$ jets $+X$ and $\mu+$ jets $+X$ final states, the scale factors for the $W+$ light partons are consistent within uncertainties between the electron and muon channels. The small deviation of the scale factors from unity is caused by the presence of small contributions from $W+$ jet events in which the $W$ decays leptonically in the samples used for the estimation of the multijet backgrounds.

The scale factors needed for the $Z+$ light parton MC are consistent with 1 for the $Z+1-3 l p \mathrm{MC}$, but not for the $Z+0 l p \mathrm{MC}$. This difference is due to systematics that we do not account for in this analysis, e.g., uncertainties on the $Z p_{T}$ reweighting, jet energy scale and lepton ID. The total contribution of $Z \rightarrow e e$ to the $e \tau$ final state is within $10 \%$ of the expected value from the $e e$ fit. The ratio of the scale factors for the $W / Z+b \bar{b}(c \bar{c}) \mathrm{MC}$ relative to the $W / Z+$ $l p \mathrm{MC}$ obtained from the fits is consistent, within errors, with the next-to-leading-order predictions [29].

One histogram that is included in the overall fit and one check histogram that is not part of the fit are shown for each of the seven final states in Figs. 1-7. In the figures, the leading and second electron are the electrons with highest $p_{T}$ in the event and next highest $p_{T}$ in the event, with a similar definition for leading and second muons and jets.


FIG. 6 (color online). $e \tau$ final state (a) The $\Delta \phi\left(e, \mathscr{C}_{T}\right)$ fit histogram and (b) invariant mass $(e, \tau)$ check histogram.

The electron $p_{T}$ distribution in Fig. 1 shows a clear disagreement between data and simulation in this kinematic region arising from the need for a large multijet contribution at low $p_{T}$, and other variables that provide better agreement with a smaller multijet contribution. However, the discrepancy at low $p_{T}$ should not mask the


FIG. 7 (color online). $\quad \mu \tau$ final state (a) muon $p_{T}$ fit histogram and (b) invariant mass ( $\mu, \tau$ ) check histogram.


FIG. 8 (color online). Sensitivity to new physics test using the $t \bar{t}$ final state. (a) The $t \bar{t} \mathrm{MC}$ is included, yielding only minor differences between data and SM background. The statistical agreement between the data and MC for the distribution shown on inset is nearly $2 \sigma$. (b) The results of the entire analysis without the $t \bar{t} \mathrm{MC}$. In this case, SLEUTH passes the criterion of interest at 0.001 for this final state. The insets show the distribution beyond the $\sum p_{T}$ cutoff. "Other" refers to contributions too small to list, including $W+b \bar{b} \rightarrow e \nu b \bar{b}$ events, $W+c \bar{c} \rightarrow$ $\ell \nu c \bar{c}$ events, $W+l p \rightarrow \ell \nu+l p$ events, and diboson events.


FIG. 9 (color online). Distribution of discrepancies for the 117 final states relative to the SM in terms of standard deviations calculated in VISTA final state before accounting for the trials factors. The curve represents a Gaussian distribution centered at zero to guide the eye. The distribution is expected to obey Poisson statistics, which is the reason the distribution is narrower than the Gaussian.


FIG. 10 (color online). (a) The distribution of the pseudorapidity of the second jet with respect to the center of the D0 detector in the $\mu+2$ jets $+\mathscr{t}_{T}$ channel. Other contains distributions too small to list individually, $W+b \bar{b}$, diboson, $t \bar{t}$, and D-Y $+0 l p$. (b) The $\Delta \phi$ distribution between the $\mu^{+}$and the $\mathscr{E}_{T}$ for the $\mu^{+} \mu^{-}+\not{ }_{T}$ final state. Other contains distributions too small to list individually, diboson and $t \bar{t}$.
presence of new physics at high $p_{T}$, which is the main focus of this analysis.

## VII. EXCLUSIVE FINAL STATES

After determining the normalization scale factors, the seven inclusive subsets are merged to create an input file for the VISTA algorithm [8]. Each MC and background


FIG. 11 (color online). The $\sigma$ distribution for the 5543 vISTA comparisons before accounting for number of the trials. The curve represents a Gaussian distribution centered at zero to guide the eye. There are 116 distributions in the underflow bin with $\sigma \leq-10$. This is expected as histograms with KolmogorovSmirnov probabilities $>0.99999$ are rounded to 1 , and appear in the underflow bin.


FIG. 12 (color online). The discrepant distributions in the $\mu+$ 2 jets $+\not \mathscr{L}_{T}$ exclusive final state. (a) The transverse mass distribution of the $W$ boson plus second jet, (b) the $\Delta \mathcal{R}$ between the muon and the second jet, (c) the invariant mass distribution of the $\mu+$ second jet, and (d) $\Delta \eta$ between the highest $p_{T}$ jet and the second jet. Other contains distributions too small to list individually, $W+b \bar{b}$, diboson, $t \bar{t}$, and $\mathrm{D}-\mathrm{Y}+0 l p$.
event is given a weight calculated from the data based scale factors and any required corrections. The VISTA algorithm, developed by the CDF Collaboration, is a tool that performs a broad check of the agreement between data and the SM. We modified the CDF algorithm for our analysis strategy as described above. The resultant VISTA@D0 algorithm focuses on the D 0 high $p_{T}$ data to determine whether the data can be adequately described by the SM or if
significant discrepancies can be confirmed. VISTA mainly examines discrepancies that affect the overall distributions rather than narrow regions of phase space, addressing the numbers of expected events and MC/data agreement across full distributions of chosen variables.

The events are separated into homogeneous subsets of events according to the objects contained in each event, resulting in 117 exclusive final states. Examples of such exclusive final states include $\mu^{ \pm} \tau^{\mp}+2$ jets $+\mathbb{E}_{T}$, $e^{ \pm} \mu^{\mp}+2$ jets $+\mathbb{E}_{T}, e^{+} e^{+}+3$ jets, and $\mu+4$ jets $+\mathbb{E}_{T}$.

VISTA performs two types of checks: first, it does a normalization-only check on the number of events in each exclusive state; the goodness of the fit is calculated using Poisson probabilities. Second, it calculates a Kolmogorov-Smirnov statistic (and resulting fit probability) for the consistency of all the kinematic distributions in any final state with the predicted SM distributions. Both of these results require additional interpretation because of the large number of trials (number of final states and/or the number of distributions) involved. When observing many final states, some disagreement is expected from statistical fluctuations in the data. Thus the Poisson probability used
to determine agreement is corrected to reflect this multiple testing. A similar effect occurs when comparing kinematic distributions, and again the probabilities are first converted to standard deviations and then corrected for the number of distributions examined.

Another algorithm we use to search for new physics is called SLEUTH [5], used at D0 for the analysis of the data collected during Run I (1992-1996) of the Tevatron. SLEUTH is an attempt to systematically search for new physics as an excess at the largest values of $\sum p_{T}$. This variable corresponds to the sum of the values of the scalar $p_{T}$ of all objects in the event, including the $\mathbb{E}_{T}$. The SLEUTH algorithm is quasi-model-independent, where "quasi" refers to the assumption that the physics beyond the SM will appear as an excess of events in some final state at large $\sum p_{T}$.

For SLEUTH, the VISTA exclusive $X+0$ jet and $X+1$ jet final states are merged, as are the $X+2$ jets and $X+3$ jets final states, and light-lepton universality is assumed, combining $e X$ and $\mu X$ channels. Underlying these assumptions is the belief that any new physics will leave similar signatures in events with no radiative jets or one radiative jet,


FIG. 13 (color online). The discrepant distributions in the $\mu+1$ jet $+\mathbb{E}_{T}$ exclusive final state: (a) the $p_{T}$ of the $W$ boson, (b) the sum of the scalar values of $p_{T}$ of the $\mu$, jet, and $\mathscr{k}_{T}$, (c) the transverse mass of the $\mu$ and $\mathscr{t}_{T}$, (d) the $p_{T}$ of the $\mu$, and (e) the $\Delta \phi$ between the muon and the jet. Other contains distributions too small to list individually, $W+b \bar{b}$, diboson, $t \bar{t}$, and $\mathrm{D}-\mathrm{Y}+0 l p$.
and in electron and muon final states. Therefore combining these final states increases the statistics in each final state while reducing the trials factor needed to account for looking in multiple final states. In each final state, the $\sum p_{T}$ distribution is scanned to find the cutoff above which the significance of any excess in data relative to the SM background is maximal, with the condition that at least three events be observed above the cutoff. This defines the most interesting region for this final state. Next, pseudoexperiments are generated with pseudo data pulled from the SM background expectation for this final state, and the fraction of pseudoexperiments is determined in which the most interesting region is at least as interesting as the most interesting region found in real data. This gives the probability that the most significant excess observed in the considered final state arise from a background fluctuation. Finally, a corrected probability is estimated from the fraction of hypothetical experiments that would produce a region in any final state at least as interesting as the most interesting region observed among all final states in real data. We define a significant output from SLeuth as one with a corrected probability of $<0.001$ (that is over 3 Gaussian standard deviations from the SM prediction using a one-sided confidence interval).

## VIII. SENSITIVITY TEST

To check the sensitivity of a search with SLEUTH, we examine whether a top quark (produced in $t \bar{t}$ pairs) which contributes objects with high $p_{T}$ would have been discovered in the current data sample. For this test, we used all the background samples, except for the $t \bar{t} \mathrm{MC}$. The main concern is whether other final states would compensate for the missing $t \bar{t}$ events, and thus SLEUTH would not be sensitive to $t \bar{t}$ production in data.

We examine the $\ell j j b \bar{b} \mathscr{C}_{T}$ final state, which we expect to be dominated by $t \bar{t}$ events. Figure 8 shows that presence or absence of a $t \bar{t}$ signal has a great impact. With a threshold of 0.001 , the SLEUTH test, including the $t \bar{t} \mathrm{MC}$, yields a statistical probability of compatibility of 0.98 after correcting for the number of trials. However, without the $t \bar{t}$ contribution this probability is $<1.1 \times 10^{-5}$. In Fig. 8 and other SLEUTH plots, the insets show the results for data and MC that pass the $\sum p_{T}$ cut maximizing the significance of excess in data.

## IX. RESULTS

## A. Numerical discrepancy using the VISTA analysis

In VISTA, the separation of the input data into final states completely defined by the objects in an event, yields a total of 117 unique exclusive final states. The probability $(\tilde{\mathcal{P}})$ that the yield observed in data results from a statistical fluctuation of the SM sample in channel $f_{s}$ is determined from

$$
\begin{equation*}
\tilde{\mathcal{P}}=1-\left(1-p_{f s}\right)^{N_{f s}} \stackrel{p_{f s} \ll 1}{\approx} N_{f s} \times p_{f s} \tag{2}
\end{equation*}
$$

where $N_{f s}$ is the number of trials and $p_{f s}$ is the probability that the number of events predicted for the channel $f_{s}$ in the SM would fluctuate to what is observed in data, before applying the correction for the number of trials. The number of trials is $N_{f s}=117$, corresponding to the number of final states, and

$$
\begin{equation*}
p_{f s}=\int_{0}^{\infty} \exp \left[-\frac{\left(N-N_{B}\right)^{2}}{2 \sigma_{B}^{2}}\right] d N \sum_{N_{\text {data }}}^{\infty} \frac{N^{i}}{i!} e^{-N} \tag{3}
\end{equation*}
$$

where $N_{B}$ and $\sigma_{B}$ are the expected SM event yield from background and its uncertainty, respectively, and $N_{\text {data }}$ is the number of events observed in any channel. The Gaussian significance is the value of $\sigma$ that satisfies the equation


FIG. 14 (color online). The discrepant histograms in the $e+$ 2 jets $+\mathscr{E}_{T}$ exclusive final state. (a) The $\Delta \eta$ between the two jets, (b) the transverse mass of the trailing jet and $\mathscr{E}_{T}$, and (c) the transverse mass distribution of the $W$ boson plus trailing jet. Other contains distributions too small to list individually, diboson, D-Y, and $t \bar{t}$.


FIG. 15 (color online). The discrepant distributions in the $e+$ 1 jet $+\mathscr{E}_{T}$ exclusive final state. (a) The $\Delta \phi$ between the $e$ and $\mathscr{E}_{T}$, (b) the $p_{T}$ of the electron, (c) the $p_{T}$ of the $W$ boson, and (d) the $\mathscr{E}_{T}$ distribution. Other contains distributions too small to list individually, diboson, D-Y, and $t \bar{t}$.

$$
\begin{equation*}
\int_{\sigma}^{\infty} \frac{1}{\sqrt{2 \pi}} e^{-\left(x^{2}\right) /(2)} d x=\tilde{\mathcal{P}} \tag{4}
\end{equation*}
$$

The final-state probabilities converted into standard deviations, before the correction factor for the number of trials, are shown in Fig. 9. This distribution shows most final states near $\sigma=0$, with some excess for $\sigma>3$. Of the 117 final states, two show significant discrepancy after correction for the number of trials. These are the final states $\mu+$

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TABLE IV. The full list of VISTA results with discrepant distributions listed by final state.

| vISTA Final state | Kinematic Variable | $\sigma$ |
| :---: | :---: | :---: |
| $\mu^{ \pm}+2$ jets $+\mathscr{E}_{T}$ | $M_{T}\left(W, j_{2}\right)$ | 4.4 |
|  | $\Delta \mathcal{R}\left(\mu, j_{2}\right)$ | 4.4 |
|  | $M\left(\mu, j_{2}\right)$ | 4.0 |
|  | $\Delta \eta\left(j_{1}, j_{2}\right)$ | 3.8 |
| $\mu^{ \pm}+1$ jet $+\not \mathbb{E}_{T}$ | $p_{T}(W)$ | 8.1 |
|  | $\Sigma p_{T}$ | 5.1 |
|  | $p_{T}(\mu)$ | 4.1 |
|  | $M_{T}\left(\mu^{ \pm}, \mathbb{E}_{T}\right)$ | 4.1 |
|  | $\Delta \phi(\mu, j)$ | 3.1 |
| $e^{ \pm}+2$ jets $+\mathbb{E}_{T}$ | $\Delta \eta\left(j_{1}, j_{2}\right)$ | 4.2 |
|  | $M_{T}\left(j_{2}, \not \mathscr{L}_{T}\right)$ | 4.0 |
|  | $M_{T}\left(W, j_{2}\right)$ | 3.0 |
| $e^{ \pm}+1 \mathrm{jet}+\underline{E}_{T}$ | $\Delta \phi\left(e^{+}, j\right)$ | 5.5 |
|  | $p_{T}\left(e^{ \pm}\right)$ | 4.4 |
|  | $p_{T}(W)$ | 3.8 |
|  | $\not{ }_{L}{ }_{T}$ | 3.1 |

2 jets $+\mathbb{E}_{T}$, with a probability corresponding to a $4.5 \sigma$ discrepancy, and $\mu^{+} \mu^{-}+\mathbb{Z}_{T}$ with a discrepancy of $6.7 \sigma$ (also shown in Fig. 9).

The discrepancy for the $\mu+2$ jets $+\mathbb{E}_{T}$ final state shows the greatest difference from the SM prediction in the modeling of jet distributions. There is a significant excess in the number of jets at high $|\eta|$, which points to likely problems with modeling initial-state-radiation/final-state-radiation jets in the forward region, as can be seen in Fig. 10(a). This difference is observed in dedicated analyses [31], and the discrepancy becomes less severe when using SHERPA [32] MC events.

The $\mu^{+} \mu^{-}+\not \mathbb{E}_{T}$ discrepancy can be attributed to difficulties modeling the muon momentum distribution for high $p_{T}$ muons. As noted in Sec. IV B 6, the muon smearing modeling is based on muons from $Z$ and $J / \psi$ decays, dominated by muons below 60 GeV , and is not as reliable at high $p_{T}$. The prime signature of poorly simulated high $p_{T}$ muons is an excess of $\not \mathscr{L}_{T}$ because of the mismodeling of the resolution of the mismeasured track. The $\Delta \phi$ between


FIG. 16 (color online). Check of most discrepant CDF plots from [9], $\mu^{ \pm} e^{ \pm}$. The inset shows the distribution above the $\Sigma p_{T}$ cut.


FIG. 17 (color online). Check of most discrepant CDF plots from [9], $\mu^{ \pm} e^{ \pm}+\mathbb{E}_{T}$. The inset shows the distribution above the $\Sigma p_{T}$ cut.
the positive muon and $\mathscr{E}_{T}$ in the $\mu^{+} \mu^{-}+\mathbb{E}_{T}$ final state is shown in Fig. 10(b), where the excess tends to be for events where the $\mathscr{Z}_{T}$ is collinear with a muon.

## B. VISTA Shape analysis of discrepancies in distributions

The 117 final states contribute a total of 5543 individual one-dimensional distributions in various variables, and comparison between simulation and data is performed for each. The trials-factor adjusted probability is determined from $\tilde{\mathcal{P}}=1-\left(1-p_{\text {shp }}\right)^{5543}$, where $p_{\text {shp }}$ is the Kolmogorov-Smirnov probability to observe a discrepancy for any individual distribution (before applying the correction for 5543 trials). As with the probability for a final-state normalization discrepancy in any final state, the probability for a discrepancy in a spectrum is converted into units of standard deviation. Any deviation $>3 \sigma$ is considered discrepant. The distribution of deviations before correction for the number of trials is shown in Fig. 11.

Sixteen distributions are found to be discrepant at the $3 \sigma$ level after correcting for the trials. The majority of these are related to spatial distributions involving jets. All these discrepancies are related to known simplifications in our modeling assumptions, e.g., no systematic uncertainties taken into account, aside from the adjustments made by the normalization factors. These discrepancies would not


FIG. 18 (color online). Check of most discrepant CDF plots from [9], $\ell^{ \pm} \ell^{\mp} \ell^{\prime}+\mathscr{E}_{T}$. The inset shows the distribution above the $\Sigma p_{T}$ cut.


FIG. 19 (color online). Since there are no data events in the $\mu^{ \pm} e^{ \pm}+2$ jets $+\mathscr{E}_{T}$ final state, the distribution for $\mu^{ \pm} e^{\mp}+$ 2 jets $+\mathscr{E}_{T}$ is shown. The inset shows the distribution above the $\Sigma p_{T}$ cut. Other contains the $Z \rightarrow \mu \mu$ and $W / Z+b \bar{b}$ distributions.
be expected to severely affect the SLEUTH search for new physics at high $p_{T}$ tails. All 16 discrepant distributions are shown in Figs. 12-15 and are listed in Table IV. In the figures, the second jet refers to the lower $p_{T}$ jet in the two jet final states.

## C. SLEUTH

All VISTA final states are used as input to Sledth, and the 117 inclusive final states are folded into 31 final states after applying global charge conjugation invariance, rebinning in the number of jets, and assuming light lepton universality. The two VISTA final states that show broad numerical excesses are found again with the SLEUTH algorithm, as expected. No additional final states have a significant SLEUTH output, as defined in Sec. VII.

In the SLEUTH runs performed at CDF, using a slightly different analysis strategy, the four most interesting observed final states were $\mu^{ \pm} e^{ \pm}, \mu^{ \pm} e^{ \pm}+2$ jets $+\mathbb{E}_{T}$, $\mu^{ \pm} e^{ \pm}+\mathbb{E}_{T}$, and $\ell^{ \pm} \ell^{\mp} \ell^{\prime}+\mathscr{E}_{T}$ in $2.0 \mathrm{fb}^{-1}$ [9] of integrated luminosity. These states were also among the most

TABLE V. The sLeuth states with $\tilde{\mathcal{P}}<0.99$. The value of $\mathcal{P}$ represents the corresponding probability without taking into account the trial factor.

| Final state | $\mathcal{P}$ | $\tilde{\mathcal{P}}^{\mathrm{a}}$ |
| :---: | :---: | :---: |
| $\ell^{+} \ell^{-}+\not \mathbb{Z}_{T}$ | $<10^{-5}$ | $<0.001$ |
| $\ell^{ \pm}+2 j+\not \mathbb{Z}_{T}$ | $<10^{-5}$ | $<0.001$ |
| $\ell^{ \pm}+\tau^{\mp}+\not \mathbb{Z}_{T}$ | $8.9 \times 10^{-5}$ | 0.0050 |
| $\ell^{ \pm}+\not \mathbb{Z}_{T}+1 j$ | 0.00036 | 0.019 |
| $e^{ \pm} \mu^{\mp}+2 b+\not \mathbb{Z}_{T}$ | 0.0028 | 0.12 |
| $\ell^{ \pm} \tau^{ \pm}+2 j+\not \mathbb{E}_{T}$ | 0.0028 | 0.12 |
| $\ell^{ \pm}+2 b+\not \mathbb{E}_{T}$ | 0.0077 | 0.3 |
| $e^{ \pm} \mu^{\mp}+\not \mathbb{Z}_{T}$ | 0.0081 | 0.31 |
| $\ell^{ \pm} \tau^{ \pm}$ | 0.057 | 0.91 |
| $\ell^{ \pm}+2 b+2 j+\not \mathbb{Z}_{T}$ | 0.099 | 0.98 |

${ }^{a}$ The value of $\tilde{\mathcal{P}}$ is not necessarily accurate below 0.001 . The important check is whether the value drops below the threshold. Further discussion can be found in [8].


FIG. 20 (color online). Distribution of final state SLEUTH probabilities converted into units of $\sigma$ before inclusion of the finalstate trials factor.
discrepant observed by CDF in $0.9 \mathrm{fb}^{-1}$ [8] of integrated luminosity. Our results for these states are shown in Figs. $16-18$, except for $\mu^{ \pm} e^{ \pm}+2$ jets $+\boldsymbol{E}_{T}$, for which we find no events with 0.16 events expected. Figure 19 shows a related final state, where the muon and electron are of opposite sign rather than of the same sign where CDF sees a discrepancy. None of these states are significantly discrepant in our analysis.

The SLEUTH final states with $\tilde{\mathcal{P}} \leq 0.99$ are shown in Table V. A plot including all of the final-state probabilities converted to units of $\sigma$ can be seen in Fig. 20. The final state $\ell^{ \pm}+\tau^{\mp}+\mathbb{E}_{T}$, which was not identified as having a significant discrepancy between data and the SM in VISTA, falls close to our SLEUTH threshold. Figure 21 shows the $\sum p_{T}$ distribution for this final state.

## X. CONCLUSIONS

We have performed a global study of D 0 high $p_{T}$ data to search for significant deviations from the standard model. This broad search for beyond standard model physics is based on $1.1 \mathrm{fb}^{-1}$ of integrated luminosity collected in Run II of the Fermilab Tevatron Collider in the D0 experiment. Using the VISTA algorithm, a total of 117 exclusive final states and 5543 kinematic distributions were compared to the SM background predictions. Only two out of 117 exclusive final states, $\mu^{ \pm}+2$ jets $+\mathscr{E}_{T}$ and $\mu^{+} \mu^{-}+$


FIG. 21 (color online). SLEUTH plot for $\ell^{ \pm}+\tau^{\mp}+\not \mathscr{L}_{T}$. The inset shows the distribution above the $\Sigma p_{T}$ cut. Other includes D-Y ee + jet events, $\mathrm{D}-\mathrm{Y} \mu \mu+$ jet events, diboson events, and $t \bar{t}$ events.
$\boldsymbol{E}_{T}$, show a statistically significant discrepancy. Given the known modeling difficulties in both final states together with our neglect in this study of systematical uncertainties, we cannot attribute the observed discrepancies to sources of physics beyond the standard model. A quasi-modelindependent search for new physics was also performed using the algorithm SLEUTH by looking for statistically significant excess at high $\sum p_{T}$ in a wide array of exclusive final states. No additional final states cross the discovery threshold in SLEUTH beyond the excesses noted by VISTA.

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## 4. $\mathrm{NO} \nu \mathrm{A}$

### 4.1 Introduction

The NuMI Off-axis $\nu_{e}$ Appearance ( $\mathrm{NO} \nu \mathrm{A}$ ) experiment is a long baseline neutrino oscillation experiment instantiated in a two-detector configuration designed to use the NuMI beamline at Fermilab to measure $\nu_{\mu} \rightarrow \nu_{e}, \bar{\nu}_{\mu} \rightarrow \bar{\nu}_{e}, \nu_{\mu} \rightarrow \nu_{\mu}$ and $\bar{\nu}_{\mu} \rightarrow \bar{\nu}_{\mu}$ transitions for neutrino energies and detector separations in the so-called "atmospheric regime." NO $\nu$ A has a particularly rich physics scope. Interaction ("appearance") rates of of $\nu_{e}$ and $\bar{\nu}_{e}$ permit a determination of the neutrino "mass hierarchy," i.e., whether the third Standard Model neutrino mass eigenstate $\nu_{3}$ is more or less massive than the other two; measure the amount of $C P$ violation in the neutrino sector by measuring the $C P$ phase angle $\delta$; measure the size of the PMNS mixing matrix angle $\theta_{13}$; and determine if the mass eigenstate $\nu_{3}$ couples more strongly to $\nu_{\mu}$ or to $\nu_{\tau}$ by measuring if the PMNS mixing matrix angle $\theta_{23}$ exceeds or is less than $\frac{\pi}{4}$, respectively. Recent $\bar{\nu}_{e}$ reactor results showing that the measured value of $\theta_{13}$ is relatively large, $\theta_{13} \simeq 9^{\circ}$, implies substantial appearance rates for $\mathrm{NO} \nu \mathrm{A}$. Additionally, measurements of $\bar{\nu}_{\mu}$ and $\nu_{\mu}$ interaction rates ("disappearance rates") permit improved precision in the measurements of the atmospheric oscillation parameters $\theta_{23}$ and $\left|\Delta m_{\mathrm{atm}}\right|$.

### 4.2 Detector Alignment

Measurements of $\mathrm{NO} \nu \mathrm{A}$ of higher level physics quantities like the $\nu_{\mu} \rightarrow \nu_{e}$ oscillation probability clearly depend on algorithms for pattern recognition, shower shape reconstruction, event selection, etc. These algorithms, in turn, rely on a knowledge of the 3 -space position of "hit" cells where energy is deposited. Incorrect hit cell positions will introduce systematic errors to things like event selection efficiency and electromagnetic shower shape reconstruction that will, in turn, propagate to the final systematic error in the higher level physics quantity of interest. Knowledge of the 3 -space position of the 350 k channels of $\mathrm{NO} \nu \mathrm{A}$ 's far detector is essential and SMU was at the core of the effort to measure these positions.

The lead worker for alignment studies at SMU was postdoc Vladimir Kravtsov who joined SMU in mid-November 2011 and is stationed full-time at Fermilab. Kravtsov focused on developing algorithms for in-situ measurements of the curvature and relative alignment of the 15 m long cells within a plane as a far detector block is built. The raw data is created using a cw "phase-based" 3-dimensional laser scanner (Leica HDS6100) that emits amplitude modulated $\sim 670 \mathrm{~nm}$ laser light in fixed spherical coordinate steps $\Delta \phi$ and $\Delta \theta$. The laser light strikes the horizontal modules, reflects back toward the scanner and the phase difference between the transmitted and reflected light is a measure of the distance between the scanner and module surface. Since the laser light is emitted uniformly in solid angle while the non-planar module surface is at varying distances from the scanner, the resulting "point cloud" of measured points on a module surface is somewhat complicated. The gist of Kravtsov's algorithm is to convert the point cloud into a non-uniform mesh
of elevation versus position in a reference plane and search for local maxima that correspond to the flat horizontal portions of a module's top surface. The centers of these portions are directly above the corresponding cell centers, the geometrical quantity of interest. Fig. 1 shows the cross section of a 32 -channel module and Fig. 2 shows several modules on the assembly table being assembled into a plane. The laser scanner is well above the assembly table, out of view.

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Figure 1: Cross-sectional view of a 32-cell module showing the non-planar top and bottom surfaces between cells. The relatively narrow top flat surfaces of a module are searched for to locate the cell centers beneath them.


Figure 2: A partial plane of modules on the assembly table at the Ash River site. The laser scanner used to measure the surface features of the modules is attached to the ceiling, out of view.


Figure 3: Measured cell curvature for 3 neighboring cells in a module. Note the consistent shape for each cell and appropriate pitch between cells, consistent with the manufacturing technique at the extrusion factory.

Kravtsov's algorithm is efficient at measuring the in-plane curvature of a module. Averaging over 50 cm contiguous sections of each 15 m long cell allows cell curvature to be measured with good statistical precision. Since cells are constrained to be physically connected to their neighbors within a module, a simple quadratic fit for in-plane curvature is sufficient. Fig 3 show results for 3 neighboring cells in a particular module. A clear banana shape is seen for each cell and the curvature
has the same sense. The distance between curves is completely consistent with the $\sim 4 \mathrm{~cm}$ cell-to-cell separation measured at the extrusion factory.

After the in-plane and out-of-plane curvatures are measured for a cell, it will be possible to describe the trajectory of a cell's center along its length by an appropriate curve. The parameters of this curve will be stored in a database for later reading during event reconstruction to better estimate the true location of hits cells. The current algorithm, developed with prototype detectors, is now automated and an automated system for transferring raw laser scan data to Fermilab for those cells in blocks under construction at Ash River is now established.

### 4.3 Monte Carlo Production Site

T. Coan, with the assistance of postdoc V. Kravtsov and FNAL computing professionals, made signficiant progress in establishing SMU as a Monte Carlo (MC) production site that would be the first such university site within $\mathrm{NO} \nu \mathrm{A}$ and so serve as a computing model for other $\mathrm{NO} \nu \mathrm{A}$ university sites. SMU has a non-trivial amount of computing resources, $\sim 1800$ cores with the Intel chipset Xeon E5540 and 6 GB of RAM/core plus an associated Lustre file system of 340 TB capacity, that is available for opportunistic use. (The SMU ATLAS group is also a user of these resources.) Equally important, its computing facility is a member of Open Science Grid and runs the 64-bit Linux operating system, making interaction with it relatively straightforward for $\mathrm{NO} \nu \mathrm{A}$. Additionally, the facility has administrative support fully paid for by SMU , so there is no burden to NO $\nu \mathrm{A}$. Our goal was to be able to submit batch MC generation jobs via the grid using standard $\mathrm{NO} \nu \mathrm{A}$ job submission procedures, have them run at SMU, and then either transfer the data back to FNAL or store them locally at SMU, whichever is more sensible for the particular job. Coan has negotiated a processing allotment of $\sim 2 \mathrm{M}$-cpu hours annually for $\mathrm{NO} \nu \mathrm{A}$, corresponding to approximately 280 cores running continuously. This level corresponds to the current (late 2012) NO $\nu \mathrm{A}$ activity on Fermigrid.

In late 2012, effort was focused on the installation of the CERN Virtual Machine File System (CVMFS) for $\mathrm{NO} \nu \mathrm{A}$ software on the SMU cluster. This was perhaps the last major step before getting SMU Monte Carlo production operational. This scheme allows the running of NO $\nu \mathrm{A}$ software on local machines from a central server without having to actually install the software locally, thereby reducing software maintenance overhead enormously. SMU hired a second systems administrator for its research computing cluster, at no cost to $\mathrm{NO} \nu \mathrm{A}$ or the SMU physics department, in mid-October 2012. This helps to ensure purely technical issues (e.g., hardware disruptions, firewall issues, kernel upgrades on local machines, etc.) are resolved efficiently. Finally, Coan purchased 96 TB of disk space to be integrated into the SMU cluster to support generation of Monte Carlo events for $\mathrm{NO} \nu \mathrm{A}$-wide use.

### 4.4 Outfitting at Ash River

T. Coan, at the request of $\mathrm{NO} \nu \mathrm{A}$ project management, was asked to be one of the physicists responsible for overseeing the outfitting of the far detector hall at Ash River and was on-site from mid-May through the end of July 2012. In conjunction with the NO $\nu$ A deputy project manager, this task involved coordinating and overseeing myriad jobs relating to such tasks as the installation of the APD cooling system, cabling for the various readout racks (high voltage, low voltage and network), module optical connector measurements and laser scanner data transmission. Although this effort is not tied directly to the development of specific data analysis code, it provides a useful, detailed overview of detector construction that may prove essential for later uncovering sources of systematic errors once data taking begins.

### 4.5 Management of the Calibration and Alignment Group

T. Coan is one of the co-convenors for the calibration and alignment group. This is a leadership position responsible for developing and managing a coherent effort to align the cells of $\mathrm{NO} \nu \mathrm{A}$ 's near and far detectors, calibrate the energy response of all cells, and monitor and correct for time dependent variations of detector response at various levels of granularity. Multiple university and national lab groups have workers in this group involved in efforts to user laser scan and cosmic ray data for detector cell alignment, to use stopping muons and muon $\mathrm{dE} / \mathrm{dx}$ to provide an energy calibration for cells, to use cosmic muons for normalizing cell-to-cell response, efforts to measure APD response linearity and threshold effects, algorithm development for $\pi^{0}$ mass peak and width measurements as a tool to check for time variations in the higher level detector response, etc. Work on developing special calibration triggers was also started. Although the group made considerable, development of the full suite of software necessary to calibrate and align the first data was still ongoing in late 2012 and early 2013.

## 5) SMU Theory: DoE Research Report:

## Fredrick Olness:

Olness works in the general area of Parton Distribution Functions (PDFs) and heavy quarks. He currently serves as co-spokesperson of the CTEQ collaboration, is a member of the International Advisory Committee for the Deep Inelastic Scattering (DIS) Workshop series, and is on the Steering Committee of the LHC-Theory Initiative. Olness also served on the organizing committee for the CTEQ/LPC Workshop (Fermilab, November 2011) and the Fall 2011 Texas-APS Meeting (Texas-A\&M, Commerce, October 2011). Within CTEQ, he has organized and/or lectured at the past six CTEQ Summer Schools, including presenting the four introductory lectures at the 2010 CTEQ-MCnet Summer school. He also was the "Theorist of the Week" (DESY, March 2010), was invited to present at the "Atlas Workshop of the Americas" (UT-Arlington, August 2010). Locally, Olness is active with the SMU Physics QuarkNet program, and serves as the Co-Director of the Dallas Regional Science Fair.

- PDFs and Nuclear Target Corrections: Refs. [1, 2, 3, 4, 5, 6, 7, 8, 9]

The Parton Distribution Functions (PDFs) are the essential ingredient which allow us to predict and interpret hadronic processes at fixed-target experiments, HERA, RHIC, Tevatron, and the LHC. In our first series of studies, we fit the charged and neutral current DIS processes separately, and extracted the nuclear correction factor for each data set. Specifically, we found that the nuclear corrections dictated by the separate charged and neutral data were quite different.[2, 3] The result of this global analysis yields the PDFs for the proton and for all nuclear A values. We have released the full set of nCTEQ PDFs used in the above studies, and these are available on-line at the HepForge repository. We have produced 19 separate PDF sets, each with 19 different nuclear A values for a total of 361 PDF sets.

- W/Z Production at the LHC and the Strange PDF: Refs. [10, 5]

At the LHC, $W$ and $Z$ boson production are used as "benchmark" processes to calibrate the decay modes of the newly discovered Higgs boson, and to search for "new physics" signatures. Motivated by questions from members of the ATLAS Standard Model group, we examined the influence of the strange quark PDF on these processes. At the LHC, the strange contribution to the $W / Z$ production processes can be as large as $30 \%$; hence a large uncertainty in the strange quark can degrade the precision these benchmark measurements. Additionally, we observed that because the $u, d$-valence quarks yield a different rapidity distribution from the $s$-quarks, an accurate measurement of the $W / Z$ could constrain the relative mix of valence and sea PDFs. Our study was published in Refs. [10, 5], and some of this work was also presented at the 2010 Atlas Workshop of the Americas held at UT-Arlington.

- Extending to Higher Order Calculations: Refs. [11, 12, 13, 14, 15, 16]

The H1 and Zeus collaborations have joined forces to produce the HERA-PDF series of proton structure fits with improved precision and reduced systematic errors.

For the massive DIS calculation, we have the complete results out to NLO, and we have used approximation methods to extend to $\mathrm{N}^{3} \mathrm{LO}$ using appropriate rescaling factors to estimate the higher order contributions. The results of this analysis were presented in Ref. [15].

- Heavy Ion Collisions at RHiC and LHC:

Ref. [17]
The LHC also has the capability to run in heavy ion mode. For example, the LHC ran with lead beams in Fall 2010, and another heavy ion run is scheduled for early 2013. In Ref. [17] we present a detailed phenomenological study of direct photon production in association with a heavy-quark jet for RHIC and LHC at NLO in QCD. This observable can provide strong constraints, over a broad $x$-range on the poorly determined nuclear parton distribution functions which are extremely important for the interpretation of results in heavy-ion collisions.

## - Model Independent Constraints on "New Physics:" <br> Refs. [18, 19]

Hadroproduction data from HERA, Tevatron, and LHC spans a broad range of energies, and these measurements can be sensitive to contributions from strongly-interacting new physics. We completed an updated QCD+SUSY global analysis on strongly interacting super-partners using the latest, most complete collider data from HERA and Tevatron to impose limits on masses of light super-partners (gluinos) as a function of $\alpha_{s}$. We find improved constraints compared to our previous (2005) study, and these limits are competitive with the best (model-independent) limits available from LEP. These limits are cited in the pdfLive (Particle Data Group) database.

- Correlated Theoretical Errors:

Ref. [20]
While at CERN, Olness and Dave Soper (U. Oregon) initiated a project to formulate the theoretical systematic uncertainties in a manner that could be numerically implemented into the global fitting analysis. The general formulation of theoretical correlated errors appears in Ref.[20].

## - Dimensional Regularization meets Freshman E\&M:

Ref. [21]
As an extension of CTEQ Summer School lectures by Olness, we developed a pedagogical example that provides an introduction to regularization, renormalization, and dimensional transmutation. This work simply elucidates renormalization scheme dependence, and the role of symmetries in a setting (a Freshman E\&M example) which is more accessible.[21].

## - Future Heavy Ion Colliders:

We proposed a new measurement at a future Electron-Ion Collider (EIC) that could clarify existence of the hypothetical "intrinsic" mechanism for charm quark production. This measurement relies on observation of charmed mesons in neutral-current DIS at large Bjorken $x$ and momentum transfer $Q$ comparable to charm mass. Intrinsic production may enhance the rate of charm meson production by up to an order of magnitude. Thus, an EIC may be uniquely suited for verifying the intrinsic charm mechanism, in contrast to other envisioned experiments. We presented some preliminary calculations on techniques to distinguish intrinsic heavy flavor production, and investigate the unique perspective provided by such a future Electron-Ion facility.[22]

- Future facilities

Refs. [23, 24, 25]

As we plan for future experiments, many scenarios include various high-intensity neutrino experiments.[24] Ref. [23] describes the potential EW "new physics" signals, and Ref. [25] outlines the QCD issues that can be addressed at a future high-intensity neutrino experiment. Olness presented this work at a Fermilab"Wine \& Cheese" talk in October 2009.

## Olness Publications

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## 1 DOE Final Report - Hornbostel

### 1.1 Research Overview

Most of the work described in this proposal was done as part of the High Precision Quantum Chromodynamics (HPQCD) Collaboration, with members P. Lepage (Cornell), C. Davies (Glasgow), J. Shigemitsu (Ohio State), H. Trottier (Simon Fraser), R. Horgan (Cambridge), E. Follana (Zaragoza), and M. Wingate (Cambridge), along with students and postdocs. HPQCD focuses on developing and employing a variety of new tools in lattice QCD with the aim of producing a range of phenomenologically relevant calculations with accuracies to within a couple per cent. These tools include improved Lagrangians, mostly with staggered quarks, more efficient lattice perturbation theory, effective actions for nonrelativistic systems, and better fitting methods. The collaboration has and continues to determine values for fundamental quantities such as the strong coupling constant $\alpha_{s}$, spectra, quark masses, and decay constants that are among the world's most precise. A particular focus is on providing precise measurements of the strongly-interacting component of the matrix elements needed to measure and overconstrain CKM matrix elements, in order to determine this more precisely, and especially in the hope that a discrepancy will point to new phenomena.

My specific contributions have been in the early development of improved lattice actions for nonrelativistic systems, and their application to charmonium and $\Upsilon$ spectra, $\alpha_{s}$ and heavy-quark mass determinations, scale setting for $\alpha_{s}$, simulation methods for highlyimproved dynamical quarks, and the use of current correlators to extract masses and current renormalizations. Research completed under this grant includes improved calculations of masses and decay constants for charm mesons using a relativistic highly-improved action and the extension to heavier masses up to the $b$ mass, current renormalization factors used to determine $D$ and $B$-meson decay constants, and improvements in fitting methods.

### 1.2 Improved Actions and Highly-Improved Staggered Quarks (HISQ)

From the early 1990s, new tools in lattice QCD such as tadpole improvement and renormalized perturbation theory revived the use of improved actions, introduced by Symanzik. These allowed the removal of lattice spacing errors using effective interactions which are perturbatively calculable, and led to more accurate simulations at greatly reduced computational cost. Our recent implementations of improved actions for QCD use the staggeredquark formulation, which retains chiral symmetry. When combined with Symanzik improvement, this is the most accurate action available and very efficient for simulations. The most recent incarnation (HISQ) is also particularly well-suited for relativistic $c$ quarks and (almost) $b$ quarks.

In the following, I describe projects which used the HISQ action and MILC configurations to measure fundamental parameters of the Standard Model, mainly in systems with $c$ or $b$ quarks.

### 1.3 Charm Systems

We just completed an updated calculation of the mass of the $J / \psi$, its leptonic width, and radiative decay [1]. New results agree with experiment, and include $M_{J / \psi}-M_{\eta_{c}}=116.5(3.2)$, $\Gamma\left(J / \psi \rightarrow e^{+} e^{-}\right)=5.48(16) \mathrm{keV}$, and $\Gamma\left(J / \psi \rightarrow \gamma \eta_{c}\right)=2.49(19) \mathrm{keV}$. The leptonic width in particular provides a successful $2 \%$ test of QCD. New ingredients in these decay calculations are the inclusion of all three light sea quarks using MILC ASQTAD configurations for the first time, and two methods to nonperturbatively renormalize the nonconserved vector current. The first is a variation of current-current correlator method discussed elsewhere; the second is by the normalization of the vector form factor between HISQ-NRQCD mesons.

### 1.4 Current Correlators, $m_{c}$ and $m_{b}$

In Ref. [2], we used the HISQ action to update sum rule method for determining the charm quark mass by comparing high-order perturbative $\overline{\mathrm{MS}}$ current-current correlators to lattice simulations rather than experimental cross sections. We were able to extract a precise value of the $c$-quark mass $m_{c}$, as well as a competitive value for $\alpha_{s}$. In Ref. [3], we extended our correlator method to include a broad range of heavy-quark masses, from below $m_{c}$ almost to $m_{b}$. We extracted a fit for the heavy MS mass as a function of $m_{\eta_{h}}$, giving both $m_{c}^{(4)}(3 \mathrm{GeV})=0.986(6) \mathrm{GeV}$ and $m_{b}^{(5)}(10 \mathrm{GeV})=3.617(25) \mathrm{GeV}$, among the most precise values available. Simultaneously we found $\alpha_{s}^{(5)}\left(M_{Z}\right)=0.1183(7)$, consistent with our determination using plaquettes, with competitive uncertainty. This approach was successful because of the fineness of the lattice configurations from MILC, with spacings from 0.15 fm to 0.045 fm , allowing us to simulate using a relativistic action with mass close enough to $m_{b}$ to allow accurate extrapolation, as well extrapolations to the continuum. We are applying extrapolations to the $b$ in several other calculations.

## $1.5 \quad s, u$ and $d$ Masses

One of the main goals of the HPQCD collaboration is to use lattice calculations to improve the precision of the fundamental parameters of the Standard Model. Among the least well known are the light-quark masses, due to confinement. The Particle Data Group quotes errors of roughly $30 \%$. We were able recently to leverage our $1 \%$-accurate $m_{c}$, along with comparably accurate results for the ratio $m_{s} / m_{c}$ of bare masses, to improve the uncertainty for the $\overline{\mathrm{MS}}$ ratio by nearly an order-of-magnitude [4] as compared to the PDG value. In particular, $m_{c} / m_{s}=11.85(16)$, giving the $\overline{\mathrm{MS}}$ mass $m_{s}^{(3)}(2 \mathrm{GeV})=92.4(1.5) \mathrm{MeV}$. We have similar reductions in errors in a new $s$ to light-quark ratio, resulting in an averaged lightquark mass of $3.40(7) \mathrm{MeV}$. Combined with the MILC $u$ and $d$ ratio, this gives MS masses $m_{u}=2.01(14) \mathrm{MeV}$ and $m_{d}=4.79(16) \mathrm{MeV}$.

### 1.6 Light Quark Condensates

Both to improve the precision of our current correlator fits involving light quarks, and because of their intrinsic interest, we directly calculated the condensates we use for $u$ and $d$,
and separately for $s$ quarks, published in Ref. [5]. Lattice QCD provides the only method to do this from first principles, allowing us to replace phenomenological estimates with well-defined values. Using $u, d, s, c$ HISQ sea quarks, with gauge configurations provided by the MILC collaboration, we computed the first direct determination of the strange quark condensate, and converted it to a nonperturbative $\overline{\mathrm{MS}}$ condensate suitable for use in the operator product expansion, finding $-(290(15) \mathrm{MeV})^{3}$. We also obtained a new value for the corresponding light-quark condensate of $-(283(2) \mathrm{MeV})^{3}$. We will employ values for the strange- and light-quark condensates directly in our fits to correlators made from heavylight quarks in order to extract quantities such as the current renormalization needed for $D$ and $B$ meson decays.

### 1.7 Relativistic $b$ Quarks using HISQ

In previous work, we were able to extend the correlator method for extracting the charm mass and $\alpha_{s}$ using the HISQ action to heavier masses $m_{h}$, as finer lattices became available from MILC and $\left(a m_{h}\right)$ errors were reduced. By fitting moments to a function of $m_{h}$, we were able to successfully extrapolate to $m_{b}$. Using a fully relativistic action with chiral symmetry provides significant advantages in that it avoids the largest NRQCD errors from relativistic corrections and current renormalization. The cost is in spacing errors of the form $\left(a m_{h}\right)$. The newest lattices from MILC, with spacing of 0.045 fm , now allow us to work just below $m_{b}$, with minimal extrapolation errors.

We extended this technique to other $b$-quark systems. In particular, we studied systems with identical heavy quarks, with $m_{h}$ ranging from below $c$ to $b$, as well as pseudoscalar mesons which combine a variable $m_{h}$ with a mass fixed $s$ or $c$. We computed masses and decay constants as a function of $m_{h}$ for both cases. This then includes new and accurate measurements of $M_{B_{c}}=6.285(10)$, and decay constants $f_{B_{c}}=0.427(6)$ and $f_{\eta_{b}}=$ $0.667(6)$ [6]. We have applied the same method to pseudoscalar meson decay constants as a function of the heavy quark mass [7]. In particular, we have improved by a factor of three the calculation of the leptonic decay constant $f_{B_{s}}$, with an error of $2 \%$. In the same study we found agreement with experiment of $m_{B_{s}}-m_{\eta_{b}} / 2$ at the same precision, and confirmed the heavy-quark mass dependence of $f_{B_{s}}$ predicted by HQET.

### 1.8 Improved Fitting Methods

To extract continuum physical quantities such as masses and decay constants, we must fit lattice monte carlo simulation data to appropriate continuum quantities such as propagators. Significant advances in the precision of lattice simulations have required similar advances in fitting technology. Toward this end, we have invested considerable effort in developing constrained Bayesian techniques [8] and code to allow for accurate fits and efficient use of high-statistics data. For example, fits to current correlators used to obtain precise values for $\alpha_{s}, m_{b}$ and $m_{c}$ simultaneously fit nearly 90 simulation results with well over 100 fit parameters, extracting these quantities while accounting for systematic errors due to discretization, higher orders in $\alpha_{s}$, finite volume, light-quark masses, experimental input data, nonperturbative contributions and others [3]. Because such extensive fits can
be computationally time consuming, we have developed methods to accelerate and simplify them by moving parameters out of fits and into data [9].

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# Nuclear Corrections in $\boldsymbol{v} A$ DIS and Their Compatibility with Global NPDF Analyses 

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#### Abstract

We perform a global $\chi^{2}$-analysis of nuclear parton distribution functions using data from charged current neutrino-nucleus ( $\nu A$ ) deep inelastic scattering (DIS), charged-lepton-nucleus ( $\ell^{ \pm} A$ ) DIS, and the Drell-Yan (DY) process. We show that the nuclear corrections in $v A$ DIS are not compatible with the predictions derived from $\ell^{ \pm} A$ DIS and DY data. We quantify this result using a hypothesis-testing criterion based on the $\chi^{2}$ distribution which we apply to the total $\chi^{2}$ as well as to the $\chi^{2}$ of the individual data sets. We find that it is not possible to accommodate the data from $v A$ and $\ell^{ \pm} A$ DIS by an acceptable combined fit. This implies that either the twist-2 parton distribution functions in nuclei are not universal, or that higher-twist terms play a more important role in the nuclear environment and have to be taken into account.


## 1 PDFs and Nuclear Corrections

High statistics neutrino deep-inelastic scattering (DIS) experiments have generated significant interest in the literature as they provide crucial information for global fits of parton distribution functions (PDFs). The neutrino DIS data provide the most stringent constraints on the strange quark distribution in the proton, and allow for flavor decomposition of the PDFs which is essential for precise predictions of the benchmark gauge boson

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[^79]production processes at the LHC. Moreover, the neutrino experiments have been used to make precision tests of the standard model (SM) in the neutrino sector. A prominent example is the extraction of the weak mixing angle $\theta_{W}$ in a Paschos-Wolfenstein type analysis [22]. A good knowledge of the neutrino DIS cross sections is also very important for long baseline experiments of the next generation which aim at measuring small parameters of the NMS mixing matrix such as the mixing angle $\theta_{13}$ and eventually the CP violating phase $\delta$.

Due to the weak nature of neutrino interactions the use of heavy nuclear targets is unavoidable, and this complicates the analysis of the precision physics discussed above since model-dependent nuclear corrections must be applied to the data. Our present understanding of the nuclear corrections is mainly based on charged lepton-nucleus ( $\ell A$ ) DIS data. In the early 1980s the European Muon Collaboration (EMC) [2] found that the nucleon structure functions $F_{2}$ for iron and deuterium differ. This discovery triggered a vast experimental program to investigate the nuclear modifications of the ratio $R\left[F_{2}^{\ell A}\right]=F_{2}^{\ell A} /\left(A F_{2}^{\ell N}\right)$ for a wide range of nuclear targets with atomic number $A$, see Table 1. By now, such modifications have been established in a kinematic range from relatively small Bjorken $x\left(x \sim 10^{-2}\right)$ to large $x(x \sim 0.8)$ in the deep inelastic region with squared momentum transfer $Q^{2}>1 \mathrm{GeV}^{2}$. The behavior of the ratio $R\left[F_{2}^{\ell A}\right]$ can be divided into four regions: (1) $R>1$ for $x \gtrsim 0.8$ (Fermi motion region), (2) $R<1$ for $0.25 \lesssim x \lesssim 0.8$ (EMC region), (3) $R>1$ for $0.1 \lesssim x \lesssim 0.25$ (anti-shadowing region), and (4) $R<1$ for $x \lesssim 0.1$ (shadowing region), with different physics mechanisms explaining the nuclear modifications. The shadowing suppression at small $x$ occurs due to coherent multiple scattering inside the nucleus of a $q \bar{q}$ pair coming from the virtual photon [1] with destructive interference of the amplitudes [7]. The anti-shadowing region is theoretically less well understood but might be explained by the same mechanism with constructive interference of the multiple scattering amplitudes [7] or by the application of momentum, charge, and/or baryon number sum rules. Conversely, the modifications at medium and large $x$ are usually explained by nuclear binding and medium effects and the Fermi motion of the nucleons [10].

Instead of trying to address the origin of the nuclear effects, the data on nuclear structure functions can be analyzed in terms of nuclear PDFs (NPDFs) which are modified as compared to the free nucleon PDFs. Relying on factorization theorems in the same spirit as in the free nucleon case, the advantage of this approach is that the universal NPDFs can be used to make predictions for a large variety of processes in $\ell A, v A, p A$, and $A A$ collisions. In addition, the nuclear correction factors required for the interpretation of the neutrino experiments can be calculated in a flexible way, taking into account the precise observable, the nuclear $A$, and the scale $Q^{2}$. The factorization assumption in the nuclear environment is therefore a question of considerable theoretical and practical importance and global analyses of NPDFs based on $\ell A$ DIS and fixed target Drell-Yan (DY) data confirm its validity in the presently explored kinematic range.

However, in a recent analysis [17] of $\nu \mathrm{Fe}$ DIS data from the NuTeV collaboration we found that the nuclear correction factors are surprisingly different from the predictions based on the $\ell^{ \pm} F e$ charged-lepton results with important implications for global analyses of proton PDFs. This finding is not completely unexpected since the structure functions in charged current (CC) neutrino DIS and neutral current (NC) electron/muon DIS are distinct observables with different parton model expressions. From this perspective it is clear that the nuclear correction factors will not be exactly the same even for a universal set of NPDFs. Note also that some models in the literature predict differences between reactions in CC and NC DIS [6]. What is, however, unexpected is the degree to which the $R$ factors differ between the structure functions $F_{2}^{\nu F e}$ and $F_{2}^{\ell F e}$. In particular the lack of evidence for shadowing in neutrino scattering down to $x \sim 0.02$ is quite surprising.

The study in Ref. [17] left open the question, whether the neutrino DIS data could be reconciled with the charged-lepton DIS data by a better flavor separation of the NPDFs. In this letter, we address this question in the $A$-dependent framework of Ref. [16] by performing a global $\chi^{2}$-analysis of the combined data from $v A$ DIS, $\ell$ A DIS and the DY process listed in Table 1.

When combining neutrino and charged-lepton+DY data into a compromise fit, we introduce a weight parameter $w$ into the $\chi^{2}$ via:

$$
\begin{equation*}
\chi^{2}=\sum_{l^{ \pm} A \text { data }} \chi_{i}^{2}+\sum_{\nu A \text { data }} w \chi_{i}^{2} . \tag{1}
\end{equation*}
$$

The $w$ factor allows us to adjust for the different number of points in the separate data sets, and provides a parameter that interpolates between the $\nu A$ and the $\ell^{ \pm} A+\mathrm{DY}$ data. We should stress that the $\chi^{2}$ cited in Table 2 and also in the text is the standard $\chi^{2}$; Eq. (1) is only used internally in the fitting procedure. We construct a set of compromise fits with weights $w=\left\{0, \frac{1}{7}, \frac{1}{2}, 1, \infty\right\}$ and study the dependence of the result on this weight. The fit to only neutrino data, denoted $w=\infty$ in Table 2, is compatible with the results in [17]. Similarly, the fit to only charged-lepton+DY data, denoted $w=0$, agrees well with the analysis in [16].

Table 1 The DIS $F_{2}^{A} / F_{2}^{A^{\prime}}$ data sets together with DY $\sigma_{D Y}^{p A} / \sigma_{D Y}^{p A^{\prime}}$ and with neutrino DIS $d \sigma^{\nu A} / d x d y$ data sets used in the fit. The table details the specific nuclear targets, and the number of data points with kinematical cuts. References for the data sets are cited in Refs. [16,17]

| ID | $\frac{F_{2}^{A}}{F_{2}^{A^{\prime}}}$ | Experiment | \# data |
| :---: | :---: | :---: | :---: |
| 1 | $\mathrm{He} / \mathrm{D}$ | SLAC-E139 | 3 |
|  |  | NMC-95,re | 12 |
| 2 | Li/D | NMC-95 | 11 |
| 3 | Be/D | SLAC-E139 | 3 |
| 4 | C/D | EMC-88 | 9 |
|  |  | EMC-90 | 0 |
|  |  | SLAC-E139 | 2 |
|  |  | NMC-95,re | 12 |
|  |  | NMC-95 | 12 |
|  |  | FNAL-E665-95 | 3 |
| 5 | N/D | BCDMS-85 | 9 |
| 6 | Al/D | SLAC-E049 | 0 |
|  |  | SLAC-E139 | 3 |
| 7 | $\mathrm{Ca} / \mathrm{D}$ | EMC-90 | 0 |
|  |  | SLAC-E139 | 2 |
|  |  | NMC-95,re | 12 |
|  |  | FNAL-E665-95 | 3 |
| 8 | $\mathrm{Fe} / \mathrm{D}$ | BCDMS-85 | 6 |
|  |  | BCDMS-87 | 10 |
|  |  | SLAC-E049 | 2 |
|  |  | SLAC-E139 | 6 |
|  |  | SLAC-E140 | 0 |
| 9 | $\mathrm{Cu} / \mathrm{D}$ | EMC-88 | 9 |
|  |  | EMC-93 | 9 |
|  |  | EMC-93 | 9 |
| 10 | Ag/D | SLAC-E139 | 2 |
| 11 | $\mathrm{Sn} / \mathrm{D}$ | EMC-88 | 8 |
| 12 | Xe/D | FNAL-E665-92 | 2 |
| 13 | $\mathrm{Au} / \mathrm{D}$ | SLAC-E139 | 3 |
| 14 | $\mathrm{Pb} / \mathrm{D}$ | FNAL-E665-95 | 3 |
| 15 | $\mathrm{Be} / \mathrm{C}$ | NMC-96 | 14 |
| 16 | $\mathrm{Al} / \mathrm{C}$ | NMC-96 | 14 |
| 17 | $\mathrm{Ca} / \mathrm{C}$ | NMC-95 | 14 |
|  |  | NMC-96 | 15 |
| 18 | $\mathrm{Fe} / \mathrm{C}$ | NMC-95 | 14 |
| 19 | $\mathrm{Pb} / \mathrm{C}$ | NMC-96 | 14 |
| 20 | C/Li | NMC-95 | 7 |
| 21 | $\mathrm{Ca} / \mathrm{Li}$ | NMC-95 | 7 |
| 22 | $\mathrm{He} / \mathrm{D}$ | Hermes | 17 |
| 23 | $\mathrm{Kr} / \mathrm{D}$ | Hermes | 12 |
| 24 | $\mathrm{Sn} / \mathrm{C}$ | NMC-96 | 111 |
| 25 | N/D | Hermes | 19 |
| 32 | D | NMC-97 | 201 |
|  | Total: |  | 616 |
| ID | $\frac{\sigma_{D Y}^{p A}}{\sigma_{D Y}^{p A^{\prime}}}$ | Experiment | \# data |
| 26 | C/D | FNAL-E772 | 9 |
| 27 | $\mathrm{Ca} / \mathrm{D}$ | FNAL-E772 | 9 |
| 28 | $\mathrm{Fe} / \mathrm{D}$ | FNAL-E772 | 9 |
| 29 | W/D | FNAL-E772 | 9 |
| 30 | $\mathrm{Fe} / \mathrm{Be}$ | FNAL-E866 | 28 |
| 31 | W/Be | FNAL-E866 | 28 |
|  | Total: |  | 92 |
| ID | $\frac{d \sigma^{v A}}{d x d y}$ | Experiment | \# data |
| 33 | Pb | CHORUS $v$ | 412 |
| 34 | Pb | CHORUS $\bar{v}$ | 412 |
| 35 | Fe | NuTeV v | 1,170 |
| 36 | Fe | NuTeV $\bar{v}$ | 966 |
| 37 | Fe | CCFR di- $\mu$ | 44 |
| 38 | Fe | NuTeV di- $\mu$ | 44 |

Table 1 continued

| ID | $\frac{d \sigma^{\nu A}}{d x d y}$ | Experiment | \# data |
| :--- | :--- | :--- | :--- |
| 39 | Fe | CCFR di- $\mu$ | 44 |
| 40 | Fe | NuTeV di- $\mu$ | 42 |
|  | Total: |  | 3,134 |

Table 2 Summary table of a family of compromise fits

| $w$ | $l^{ \pm} A$ | $\chi^{2}(/ \mathrm{pt})$ | $\nu A$ | $\chi^{2}(/ \mathrm{pt})$ | Total $\chi^{2}(/ \mathrm{pt})$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 0 | 708 | $638(0.90)$ | - | - | $638(0.90)$ |
| $1 / 7$ | 708 | $645(0.91)$ | 3,134 | $4,710(1.50)$ | $5,355(1.39)$ |
| $1 / 2$ | 708 | $680(0.96)$ | 3,134 | $4,405(1.40)$ | $5,085(1.32)$ |
| 1 | 708 | $736(1.04)$ | 3,134 | $4,277(1.36)$ | $5,014(1.30)$ |
| $\infty$ | - | - | 3,134 | $4,192(1.33)$ | $4,192(1.33)$ |




Fig. 1 Predictions from the compromise fits for the nuclear correction factors $R\left[F_{2}^{\ell F e}\right] \simeq F_{2}^{\ell F e} / F_{2}^{\ell N}$ (left) and $R\left[F_{2}^{\nu F e}\right] \simeq$ $F_{2}^{\nu F e} / F_{2}^{\nu N}$ (right) as a function of $x$ for $Q^{2}=5 \mathrm{GeV}^{2}$. The data points displayed in figure a) are from BCDMS and SLAC experiments [3-5,8,11] and those displayed in figure b) come from the NuTeV experiment [20,21]

We first examine the nuclear correction factors $R\left[F_{2}^{F e}\right] \simeq F_{2}^{F e} / F_{2}^{N}$ needed to correct the nuclear data to the free nucleon level. ${ }^{1}$ We compute these quantities in the QCD parton model at next-to-leading order employing the NPDF fits in Table 2. The $x$-dependence of $R\left[F_{2}^{F e}\right]$ is shown in Fig. 1; similar results hold at $Q^{2}=20 \mathrm{GeV}^{2}$ which we do not present here. The $w=0$ fit uses only the $\ell A$ DIS+DY data, and this agrees well with the SLAC and BCDMS points [3-5,8,11] displayed in Fig. 1a). However, as we mix in the $v A$ data, Table 2 shows the $\chi^{2}$ of the $\ell A$ data rise from 638 for $w=0$ to 736 for $w=1$. Correspondingly, the $w=\infty$ fit uses only the $\nu A$ data, and this agrees well with the data from the NuTeV experiment $[20,21]$ displayed in Fig. 1b). Now as we mix in the $\ell A$ DIS+DY data, we see the $\chi^{2}$ of the $v A$ data rise from 4192 for $w=\infty$ to 4710 for $w=1 / 7$. Finally, comparing the results obtained with the $w=0$ and the $w=\infty$ fits one can see that they predict considerably different $x$-shapes.

The fits with weights $w=\left\{\frac{1}{7}, \frac{1}{2}, 1\right\}$ interpolate between these two incompatible solutions. As can be seen in Fig. 1a, b, with increasing weight the description of the $\ell F e$ data is worsened in favor of a better agreement with the $\nu \mathrm{Fe}$ points. This trend clearly demonstrates that the $\ell F e$ and the $\nu \mathrm{Fe}$ data pull in opposite directions. We identify the fits with $w=1 / 2$ or $w=1$ as the best candidates for a possible compromise.

To be able to decisively accept or reject the compromise fits, we apply a statistical goodness-of-fit criterion $[9,13,19]$ based on the probability distribution for the $\chi^{2}$ given that the fit has $N$ degrees of freedom:

$$
\begin{equation*}
P\left(\chi^{2}, N\right)=\frac{\left(\chi^{2}\right)^{N / 2-1} e^{-\chi^{2} / 2}}{2^{N / 2} \Gamma(N / 2)} \tag{2}
\end{equation*}
$$

This allows us to define the percentiles $\xi_{p}$ via $\int_{0}^{\xi_{p}} P\left(\chi^{2}, N\right) d \chi^{2}=p \%$ where $p=\{50,90,99\}$. Here, $\xi_{50}$ serves as an estimate of the mean of the $\chi^{2}$ distribution and $\xi_{90}$, for example, gives us the value where there is only a $10 \%$ probability that a fit with $\chi^{2}>\xi_{90}$ genuinely describes the given set of data. In a global PDF fit, the best fit $\chi^{2}$ value often deviates from the mean value because the data come from different possibly incompatible experiments having unidentified, unknown errors which are not accounted for in the experimental

[^80]systematic errors. For this reason we rescale the $\xi_{90}$ and $\xi_{99}$ percentiles relative to the best fit $\chi_{0}^{2}$ [19] to define $C_{90}=\chi_{0}^{2}\left(\xi_{90} / \xi_{50}\right)$ and $C_{99}=\chi_{0}^{2}\left(\xi_{99} / \xi_{50}\right)$. This defines our criterion: a fit with a given $\chi^{2}$ is compatible with the best fit with $\chi_{0}^{2}$ at $90 \%(99 \%)$ confidence if $\chi^{2}<C_{90}\left(\chi^{2}<C_{99}\right)$. We apply it to both the total $\chi^{2}$ and the $\chi^{2}$ of the individual data sets.

For the $\ell A$ DIS+DY data we use the fit with $w=0$ as benchmark with $\chi_{0}^{2}=638$ and $N=677$ degrees of freedom (for 708 data points and 31 free parameters). The upper limits on the $\chi^{2}$ at $90 \%$ and $99 \%$ confidence level (C.L.) are then $C_{90}^{l^{ \pm} A}=683.6$ and $C_{99}^{l^{ \pm} A}=722.2$. The benchmark fit for the $\nu A$ DIS data $(w=\infty)$ uses 3,134 data points with 33 free parameters resulting in $N=3,101$ and one finds $C_{90}^{\nu A}=4,330$ and $C_{99}^{\nu A}=4,445$. We see that none of the compromise fits satisfies both limits at the $90 \%$ C.L. which is usually used in global analyses of PDFs to define the uncertainty bands. At the $99 \%$ C.L., there are two fits ( $w=1 / 2, w=1$ ) which are below the $C_{99}^{\nu A}$ limit. However, only the $w=1 / 2$ fit satisfies the corresponding constraint from the charged-lepton benchmark fit.

We now apply our criterion also to the individual data sets with IDs between 1 and 40 in Table 1 . For the $\ell A$ DIS + DY data (ID $=[1,31]$ ) we determine the $31 C_{90}\left(C_{99}\right)$ limits by using the individual $\chi_{i}^{2}$ of the $w=0$ fit as $\chi_{0, i}^{2}$. For the $\nu A$ DIS data (ID $=[32,40]$ ) we proceed in a similar manner using the individual $\chi_{i}^{2}$ of the $w=\infty$ fit. The results of this detailed analysis are depicted in Fig. 2, where we show the quantity

$$
\begin{equation*}
\frac{\Delta \chi^{2}}{\Delta C_{90}}=\frac{\chi_{i}^{2}-\chi_{0, i}^{2}}{C_{90, i}-\chi_{0, i}^{2}} \quad(i=1, \ldots, 40) \tag{3}
\end{equation*}
$$

where $\chi_{i}^{2}$ represents the $\chi^{2}$-value of the $i$ 'th data set. In cases where $\chi_{i}^{2}>C_{90, i}$ the fit is not compatible with the best fit at the $90 \%$ level and $\Delta \chi^{2} / \Delta C_{90}>1$. The exact $90 \%$ C.L. limit is shown as a constant solid line and the dotted line represents the $99 \%$ confidence limit. The local application of the $\chi^{2}$ hypothesis-testing criterion reveals that even the compromise fit with weight $w=\frac{1}{2}$ which was considered acceptable at the $99 \%$ C.L. when looking at the nuclear correction factors and at the global change in $\chi^{2}$, cannot be accepted as a compromise solution as both the charged-lepton and neutrino DIS data on iron exceed the $99 \%$ limit.

In conclusion, the tension between the $\ell^{ \pm} F e$ and $\nu F e$ data sets leaves us with no possible compromise fit when investigating the results in detail, not even when using the $99 \%$ percentile as the limit as opposed to the more restrictive $90 \%$ limit which is usually used to construct the error PDFs. This detailed analysis confirms the preliminary conclusions of Refs. [16,17] that there is no possible compromise fit which adequately describes the neutrino DIS data along with the charged-lepton DIS and DY data.

At face value, this conclusion differs from some results in the literature which argue the $v A$ and $\ell^{ \pm} A$ data are in accord. [15] Here, we believe an essential element in our analysis is the use of the correlated systematic errors of the $\nu A$ data. To highlight this point, we now repeat our analysis, but we combine the statistical and all systematic errors in quadrature (thereby neglecting the information contained in the correlation matrix) for $v A$ data for the $w=1$ fit with $Q^{2}>4 \mathrm{GeV}^{2}$ (as before); we denote this the "Ucor4" fit, and we obtain $\chi^{2} / p t$ of 1.14 for $\ell^{ \pm} A$ and 1.00 for $v A$. We also use a $Q^{2}>5 \mathrm{GeV}^{2}$ fit (denoted "Ucor5") to mimic the cuts of Ref. [15]; here we obtain $\chi^{2} / p t$ of $721 / 633=1.14$ for $\ell^{ \pm} A$ and $2,828 / 2,947=0.96$ for $v A$.

If we examine the total $\chi^{2}$ values, we find the $\chi^{2} / \operatorname{dof} \sim 1$, and might be tempted to conclude we are able to fit both the $v A$ and $\ell^{ \pm} A$ data simultaneously. However, if we look at individual data sets and apply


Fig. $2 \Delta \chi^{2} / \Delta C_{90}$ as defined in Eq. (3) for the 40 individual data sets. Results are shown for the $w=\frac{1}{2}$-fit (left) and the fit 'Ucor5' (right) with $w=1$. The solid and dashed lines indicate the $90 \%$ and $99 \%$ confidence limits. The highlighted data sets correspond to the DIS NuTeV $\ell^{ \pm} F e(\mathrm{ID}=8), v F e(\mathrm{ID}=35)$, and $\bar{v} F e(\mathrm{ID}=36)$
our hypothesis testing criteria, the picture is quite different. Fig. 2b displays the results for the Ucor5 fit. The higher $Q^{2}$ cut of the Ucor5 fit removes some of the very precise NuTeV data at small-x, thus resulting in an improved $\chi^{2}$ compared to Ucor4. Nevertheless, many of the $\ell^{ \pm} F e$ data sets (ID $=3,4,5,6,8$ ) still lie outside the $99 \%$ CL percentile. ${ }^{2}$ Thus, we still conclude that there is no compromise fit for the $\nu A$ and $\ell^{ \pm} A$ data even if we relax the constraints by using uncorrelated errors.

Consequently, the nuclear correction factor for the neutrino DIS data are indeed incompatible with that of the charged lepton DIS and DY data, and this result depends crucially on the use of the precision correlated errors of the neutrino data. This result has important implications for both nuclear and proton PDFs. If we do not know the appropriate nuclear correction to relate different targets of nuclear $A$, our ability to extract PDFs is limited. For example, the CTEQ6.6 analysis [14] sidesteps this issue by removing most of the $\nu A$ data from the fit; however, they retain the NuTeV dimuon data since this data is critical to constraining the strange quark PDF. This underscores the importance of the $v A$ data for flavor differentiation.

Although the NuTeV data provides the tightest constraints due to their statistics, we note that this issue cannot be tied to a single data set. For example, we find that NuTeV is generally compatible with CCFR and CDHSW. ${ }^{3}$ The CHORUS $v P b$ and $\bar{\nu} P b$ data have larger uncertainties, so they can be compatible with both the $\ell^{ \pm} A$ data and the NuTeV $\nu F e$ data because the $\Delta \chi^{2} / \Delta C_{90}<1$ for all weights. Compared to the theory predictions, NuTeV agrees well in the central $x$ region, but exhibits differences both for low $x$ at low $Q^{2}$, and also for very high $x(x \sim 0.65)$.

## 2 Conclusions

We have demonstrated that the $v A$ and $\ell^{ \pm} A$ data prefer different nuclear correction factors, and that there is no single "compromise" result that will simultaneously satisfy both data sets. While we have focused on the phenomenological aspects for the present study, this result has strong implications for the extraction of both nuclear and proton PDFs using combined neutrino and charged-lepton data sets. Possibilities include unexpectedly large higher-twist effects, or even non-universal nuclear effects; we leave such questions for a future study.

## 3 nCTEQ PDF Sets Available On-line

The nCTEQ PDF sets are available on-line at the HepForge repository (http://projects.hepforge.org/ncteq/). This repository contains the 19 families of PDFs used in Refs. [12, 16, 18], and each family contains PDF grids for a range of nuclei specified by the number of nucleons $(\mathrm{A})$ and the number of protons $(\mathrm{Z})$; in total there are 361 separate nuclear PDF grids. A sample Fortan program is included to demonstrate the use of these nuclear PDF sets.

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# Nuclear parton distribution functions 

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We study nuclear effects of charged current deep inelastic neutrino-iron scattering in the framework of a $\chi^{2}$ analysis of parton distribution functions (PDFs). A set of iron PDFs are extracted and used to compute $x_{B j}$ dependent and $Q^{2}$-dependent nuclear correction factors which are required in global analyses of free nucleon PDFs. We compare our results with nuclear correction factors from neutrino-nucleus scattering models and correction factors for $\ell^{ \pm}$-iron scattering. Except for very high $x_{B j}$, our correction factors differ in both shape and magnitude from the correction factors of the models and charged-lepton scattering.

## 1. Impact of Nuclear Corrections on PDFs

The high statistics measurements of neutrino deeply inelastic scattering (DIS) on heavy nuclear targets has generated significant interest in the literature since these measurements provide valuable information for global fits of parton distribution functions (PDFs). It is necessary to use both Charged Current (CC) $W^{ \pm}$probes and Neutral Current (NC) $\{\gamma, Z\}$ probes to disentangle the separate PDF flavor components. Toward this goal, the use of nuclear targets is unavoidable due to the weak nature of the $\left\{W^{ \pm}, Z\right\}$ interactions, and this complicates the extraction of free nucleon PDFs because model-dependent corrections must be applied to the data.

In early PDF analyses, the nuclear corrections were static correction factors without any (significant) dependence on the energy scale $Q$, the atomic number $A$, or the specific observable. The increasing precision of both the experimental data and the extracted PDFs demand that the applied nuclear correction factors be equally precise as
these contributions play a crucial role in determining the PDFs.
In this study we reexamine the source and size of the nuclear corrections that enter the PDF global analysis, and quantify the associated uncertainty. Additionally, we provide the foundation for including the nuclear correction factors as a dynamic component of the global analysis so that the full correlations between the heavy and light target data can be exploited.

A recent study [1] analyzed the impact of new data sets from the NuTeV, Chorus; and E-866 Collaborations on the PDFs. This study found that the NuTeV data set (together with the model used for the nuclear corrections) pulled against several of the other data sets, notably the E-866, BCDMS and NMC sets. Reducing the nuclear corrections at large values of $x$ reduced the severity of this pull and resulted in improved $\chi^{2}$ values. These results suggest on a purely phenomenological level that the appropriate nuclear corrections for $\nu$-DIS may well be smaller than assumed.

[^82]
## 2. Global Analysis Framework

To investigate this question further, we use the high-statistics $\nu$-DIS experiments to perform a dedicated PDF fit to neutrino-iron data [2]. Since we first will study iron alone and will not (initially) combine the data with measurements on different target materials, we need not make any assumptions about the nuclear corrections; this side-steps a number of difficulties $[3,1,4]$. While this approach has the advantage that we do not need to model the $A$-dependence, it has the drawback that the data from just one experiment will not be sufficient to constrain all the parton distributions; therefore, other assumptions must enter the analysis. The theoretical framework will roughly follow the CTEQ6 analysis of free proton PDFs [5]. We outline the key features of our analysis below, and focus on the issues specific to our study of NuTeV neutrino-iron data in terms of nuclear parton distribution functions.

### 2.1. Basic formalism

For our PDF analysis, we will use the general features of the QCD-improved parton model and the $\chi^{2}$ analyses as outlined in Ref. [5]. We adopt the framework of the recent CTEQ6 analysis of proton PDFs where the input distributions at the scale $Q_{0}=1.3 \mathrm{GeV}$ are parameterized as
$x f_{i}\left(x, Q_{0}\right)=A_{0} x^{A_{1}}(1-x)^{A_{2}} e^{A_{3} x}\left(1+e^{A_{4}} x\right)^{A_{5}}$
for $i=\left\{u_{v}, d_{v}, g, \bar{u}+\bar{d}, s, \bar{s}\right\}$, and
$x f_{i}\left(x, Q_{0}\right)=A_{0} x^{A_{1}}(1-x)^{A_{2}}+\left(1+A_{3} x\right)(1-x)^{A_{4}}$
for $i=\{\bar{d} / \bar{u}\}$ where $u_{v}$ and $d_{v}$ are the up- and down-quark valence distributions, $\bar{u}, \bar{d}, s, \bar{s}$ are the up, down, strange and anti-strange sea distributions, and $g$ is the gluon. Furthermore, the $f_{i}=f_{i}^{p / A}$ denote parton distributions of bound protons in the nucleus $A$, and the variable $0 \leq x \leq A$ is defined as $x:=A x_{A}$ where $x_{A}=Q^{2} / 2 p_{A} \cdot q$ is the usual Bjorken variable formed out of the four-momenta of the nucleus and the exchanged boson. This parameterization is designed for $0 \leq x \leq 1$ and we here neglect ${ }^{2}$ the

[^83]distributions at $x>1$. Note that the condition $f_{i}(x>1, Q)=0$ is preserved by the DGLAP evolution and has the effect that the evolution equations and sum rules for the $f_{i}^{p / A}$ are the same as in the free proton case.

The PDFs for a nucleus $(A, Z)$ are constructed as
$f_{i}^{A}(x, Q)=\frac{Z}{A} f_{i}^{p / A}(x, Q)+\frac{(A-Z)}{A} f_{i}^{n / A}(x, Q)$
where we relate the distributions inside a bound neutron, $f_{i}^{n / A}(x, Q)$, to the ones in a proton by assuming isospin symmetry. The nuclear structure functions are given by parallel relations such that they can be computed in next-to-leading order as convolutions of the nuclear PDFs with the conventional Wilson coefficients, i.e., generically $F_{i}^{A}(x, Q)=\sum_{k} C_{i k} \otimes f_{k}^{A}$.

In order to take into account heavy quark mass effects we calculate the relevant structure functions in the ACOT scheme [11, 12] in NLO QCD [13]. Finally, the differential cross section for charged current (anti-)neutrino-nucleus scattering is given in terms of three structure functions:

$$
\begin{aligned}
& \frac{d^{2} \sigma}{d x d y} \stackrel{(-)}{\nu} A=\frac{G_{F}^{2} M E}{\pi}\left[\left(1-y-\frac{M x y}{2 E}\right) F_{2}^{(-)} A\right. \\
&+\frac{y^{2}}{2} 2 x F_{1}^{(-)} A \\
& \nu
\end{aligned}
$$

where the '+' ('-') sign refers to neutrino (antineutrino) scattering and where $G_{F}$ is the Fermi constant, $M$ the nucleon mass; and $E$ the energy of the incoming lepton (in the laboratory frame).

### 2.2. Methodology

The basic formalism described in the previous sections is implemented in a global PDF fitting package, but with the difference that no nuclear corrections are applied to the analyzed data; hence, the resulting PDFs are for a bound proton in an iron nucleus. The parameterization provides enough flexibility to describe current data sets entering a global analysis of free nucleon PDFs; given that the nuclear modifications of the $x$-shape appearing in this analysis are modest, this parameterization will also accommodate the iron PDFs.

Because the neutrino data alone do not have the power to constrain all of the PDF components, we will need to impose some minimal set of external constraints. For example, our results are rather insensitive to the details of the gluon distribution with respect to both the overall $\chi^{2}$ and also the effect on the quark distributions. The nuclear gluon distribution is very weakly constrained by present data, and a gluon PDF with small nuclear modifications has been found in the NLO analysis of Ref. [14]. We have therefore fixed the gluon input parameters to their free nucleon values. For the same reasons the gluon is not sensitive to this analysis, fixing the gluon will have minimal effect on our results. Furthermore, we have set the $\bar{d} / \bar{u}$ ratio to the free nucleon result assuming that the nuclear modifications to the down and up sea are similar such that they cancel in the ratio. This assumption is supported by Fig. 6 in Ref. [14].

## 3. Analysis of iron data

### 3.1. Iron Data Sets

We determine iron PDFs using the recent NuTeV differential neutrino and anti-neutrino DIS cross section data [15]. In addition, we include NuTeV/CCFR dimuon data [16] which are sensitive to the strange quark content of the nucleon. There are other measurements of neutrino-iron DIS available in the literature from the CCFR [17, 18, 19, 20]; CDHS [21] and CDHSW [22] collaborations; see, e.g., Ref. [23] for a review. There is also a wealth of charged lepton-iron DIS data including SLAC [24] and EMC $[25,26] .{ }^{3}$ For the initial study we limit our analysis to the NuTeV experiment alone; we will compare and contrast different experiments in a subsequent study.

### 3.1.1. PDF Reference Sets

For the purposes of this study, we use two different reference sets of free-proton PDFs which we denote 'Base-1' and 'Base-2'.

Since we focus on iron PDFs and the associated nuclear corrections, we need a base set of PDFs

[^84]which are essentially free of any nuclear effects; this is the purpose of the Base-1 reference set [1]. Therefore, to extract the Base-1 PDFs we omit the CCFR and NuTeV data from our fit so that our base PDFs do not contain any large residual nuclear corrections. ${ }^{4}$ The absence of such nuclear effects will be important when we extract the nuclear corrections factors.
The Base-2 PDFs are essentially the CTEQ6.1M PDFs with a modified strange PDF introduced to accommodate the NuTeV dimuon data. ${ }^{5}$ In the manner of the CTEQ6.1M PDF's, the Base-2 fit does not apply any deuteron corrections to the data; this is in contrast to the Base-1 PDFs. Also, the Base-2 fit does include the CCFR data that has been corrected to a free nucleon using charged-lepton correction factors [20].
By comparing the free-proton PDF 'Base-1' and 'Base-2' sets with the iron PDF sets, we can gauge the size of the nuclear effects. Furthermore, differences between observables using the 'Base-1' respectively the 'Base-2' reference sets will indicate the uncertainty due to the choice of the freeproton PDF.

### 3.1.2. Comparison of the Fits with Data

Specifically, we determine iron PDFs using the recent NuTeV differential neutrino ( 1371 data points) and anti-neutrino (1146 data points) DIS cross section data [15]. and we include NuTeV/CCFR dimuon data (174 points) which are sensitive to the strange quark content of the nucleon. Using the ACOT scheme, we impose kinematic cuts of $Q>2 \mathrm{GeV}$ and $W>3.5 \mathrm{GeV}$, and obtain a good fit with a $\chi^{2}$ of 1.35 per data point; we identify this fit as 'A2.'[2]

[^85]
### 3.2. Iron PDFs

We now examine the nuclear (iron) parton distributions $f_{i}^{A}\left(x, Q^{2}\right)$ in Figure 1 which shows the PDFs from fit 'A2' at our input scale $Q_{0}=m_{c}=$ 1.3 GeV versus $x$. For an almost isoscalar nucleus like iron the $u$ and $d$ distributions are very similar. Therefore, we only show the $u_{v}$ and $\bar{u}$ partons, together with the strange sea. ${ }^{6}$ As explained above, the gluon distribution is very similar to the familiar CTEQ6M gluon at the input scale such that we don't show it here. In order to indicate the constraining power of the NuTeV data, the band of reasonable fits is depicted. The fits in this band were obtained (as outlined above) by varying the initial conditions and the number of free parameters to fully explore the solution space. All the fits shown in the band have $\chi^{2} / D O F$ within 0.02 , which roughly corresponds to a range of $\Delta \chi^{2} \sim 50$ for the 2691 data points.

As can be seen in Figure 1, the $u_{v}$ distribution has a very narrow band across the entire $x$ range. The up- and strange-sea distributions are less precisely determined. At values of $x$ down to, say, $x \simeq 0.07$ the bands are still reasonably well confined; however, they open up widely in the small- $x$ region. Cases where the strange quark sea lies above the up-quark sea are unrealistic, but are present in some of the fits since this region ( $x \lesssim 0.02$ ) is not constrained by data. We have included the curves for our free-proton Base-1 PDFs (dashed), as well as the HKN04 [7] (dotted), the NLO HKN07 [8] (dotted-dashed), and DS [14] (dot-dashed) nuclear PDFs. ${ }^{7}$

The comparison with the Base-1 PDFs is straightforward since the same theoretical framework (input scale, functional form, NLO evolution) has been utilized for their determination. Therefore, the differences between the solid band

[^86]

Figure 1. Parton distributions for iron. The central PDF from fit 'A2' is shown by the solid line. The dashed lines depict parton distributions constructed according to Eq. 1 with $A=56$ and $Z=26$ using the Base- 1 free-proton PDFs. Additional results are shown from HKNO4 [7]; (NLO) HKN07 [8], and (DS) [14]. The vertical line marks the lower limit of the data in the $x$ variable.
('A2') and the dashed line (Base-1) exhibit the nuclear effects, keeping in mind that the freeproton PDFs themselves have uncertainties.

For the comparison with the HKN04 distributions, it should be noted that a $\mathrm{SU}(3)$-flavor symmetric sea has been used; therefore, the HKN04 strange quark distribution is larger, and the light quark sea smaller, than their Base-1 PDF counterparts over a wide range in $x$. Furthermore, the HKN04 PDFs are evolved at leading order.

In a recent analysis, the HKN group has published a new set of NPDFs (HKN07) including uncertainties [8]. They provide both LO and NLO sets of PDFs, and we display the NLO set. These PDFs also use a more general set of sea distributions such that $\bar{u}(x) \neq \bar{d}(x) \neq \bar{s}(x)$ in general.

The DS PDFs are linked to the GRV98 PDFs [27] with a rather small radiatively generated strange sea distribution. Consequently, the light quark sea is enhanced compared to the other sets. Additionally, the DS sets are evolved in a 3-fixedflavor scheme in which no charm parton is included in the evolution. However, at the scale $Q=m_{c}$ of Fig. 1 this is of no importance.

## 4. Nuclear Correction Factors

In the previous section we analyzed charged current $\nu-\mathrm{Fe}$ data with the goal of extracting the iron nuclear parton distribution functions. In this section, we now compare our iron PDFs with the free-proton PDFs (appropriately scaled) to infer the proper heavy target correction which should be applied to relate these quantities.

Within the parton model, a nuclear correction factor $R[\mathcal{O}]$ for an observable $\mathcal{O}$ can be defined as follows:
$R[\mathcal{O}]=\frac{\mathcal{O}[\mathrm{NPDF}]}{\mathcal{O}[\text { free }]}$
where $\mathcal{O}[\mathrm{NPDF}]$ represents the observable computed with nuclear PDFs, and $\mathcal{O}$ [free] is the same observable constructed out of the free nucleon PDFs. Clearly, $R$ can depend on the observable under consideration simply because different observables may be sensitive to different combinations of PDFs.

This means that the nuclear correction factor $R$ for $F_{2}^{A}$ and $F_{3}^{A}$ will, in general, be different. Additionally, the nuclear correction factor for $F_{2}^{A}$ will yield different results for the charged current
$\nu-F e$ process ( $W^{ \pm}$exchange) as compared with the neutral current $\ell^{ \pm}-F e$ process ( $\gamma$ exchange). Schematically, we can write the nuclear correction for the DIS structure function $F_{2}$ in a charged current (CC) $\nu-A$ process as: ${ }^{8}$
$R_{C C}^{\nu}\left(F_{2} ; x, Q^{2}\right) \simeq \frac{d^{A}+\bar{u}^{A}+\ldots}{d^{\emptyset}+\bar{u}^{\emptyset}+\ldots}$
and contrast this with the neutral current (NC) $\ell^{ \pm}-A$ process:

$$
\begin{aligned}
& \quad R_{N C}^{e, \mu}\left(F_{2} ; x, Q^{2}\right) \simeq \\
& \frac{\left(-\frac{1}{3}\right)^{2}\left[d^{A}+\bar{d}^{A}+\ldots\right]+\left(+\frac{2}{3}\right)^{2}\left[u^{A}+\bar{u}^{A}+\ldots\right]}{\left(-\frac{1}{3}\right)^{2}\left[d^{\emptyset}+\bar{d}^{\emptyset}+\ldots\right]+\left(+\frac{2}{3}\right)^{2}\left[u^{\emptyset}+\bar{u}^{\emptyset}+\ldots\right]},
\end{aligned}
$$

where the superscript " 0 " denotes the "free nucleon" PDF which is constructed via the relation:
$f_{i}^{\emptyset}(x, Q)=\frac{Z}{A} f_{i}^{p}(x, Q)+\frac{(A-Z)}{A} f_{i}^{n}(x, Q)$
Clearly, the $R$-factors depend on both the kinematic variables and the factorization scale. Finally, we note that Eq. 2 is subject to uncertainties of both the numerator and the denominator.
We will now evaluate the nuclear correction factors for our extracted PDFs, and compare these with selected results from the literature [28, 29]. ${ }^{9}$ Because we have extracted the iron PDFs from only iron data, we do not assume any particular form for the nuclear $A$-dependence; hence the extracted $R[\mathcal{O}]$ ratio is essentially model independent.

## 4.1. $F_{2}^{F e} / F_{2}^{D} \mathrm{NC}$ charged lepton scattering

We will also find it instructive to compare our results with the $F_{2}^{\mathrm{Fe}} / F_{2}^{\mathrm{D}}$ as extracted in neutral current charged-lepton scattering; $\ell^{ \pm}-F e$. In Fig. 2 we compare the experimental results for the structure function ratio $F_{2}^{\mathrm{Fe}} / F_{2}^{\mathrm{D}}$ for the following experiments: BCDMS-85 [30], BCDMS-87 [31], SLAC-E049 [32], SLAC-E139 [3], SLAC-140 [24]. The curve (labeled SLAC/NMC parameterization) is a fit to this data. While there is

[^87]

Figure 2. Parameterization for the neutral current charged lepton structure function $F_{2}^{F e} / F_{2}^{D}$. For comparison we show experimental results from the BCDMS collaboration (BCDMS-85 [30]; BCDMS-87 [31]) and from experiments at SLAC (SLAC-E049 [32], SLAC-E139 [3], and SLACE140 [24]). Normalization uncertainties of the data have not been included.
a spread in the individual data points, the parameterization describes the bulk of the data at the level of a few percent or better. It is important to note that this parameterization is independent of atomic number $A$ and the energy scale $Q^{2}$ [33]; this is in contrast to the results we will derive using the PDFs extracted from the nuclear data. ${ }^{10}$ Additionally, we note that while this parameterization has been extracted using ratios of $F_{2}$ structure functions, it is often applied to other observables such as $F_{1,3, L}$ or $d \sigma$. We can use this parameterization as a guide to judge the approximate correspondence between this neutral current (NC) charged lepton DIS data and our charged current (CC) neutrino DIS data.

### 4.2. R Factors for $d^{2} \sigma / d x d Q^{2}$

We begin by computing the nuclear correction factor $R$ according to Eq. (2) for the neutrino differential cross section as this represents the bulk

[^88]

Figure 3. Nuclear correction factor $R$ for the differential cross section $d^{2} \sigma / d x d Q^{2}$ in charged current neutrino-Fe scattering at $Q^{2}=5 \mathrm{GeV}^{2}$. Results are shown for the charged current neutrino (solid lines) and anti-neutrino (dashed lines) scattering from iron. The upper (lower) pair of curves shows the result of our analysis with the Base-2 (Base-1) free-proton PDFs.
of the NuTeV data included in our fit. More precisely, we show $R$-factors for the charged current cross sections $d^{2} \sigma / d x d Q^{2}$ at fixed $Q^{2}$. Our results are displayed in Fig. 3 for $Q^{2}=5 \mathrm{GeV}^{2}$ and a neutrino energy $E_{\nu}=150 \mathrm{GeV}$ which implies, due to the relation $Q^{2}=2 M E_{\nu} x y$, a minimal $x$ value of $x_{\text {min }}=0.018$. The solid (dashed) lines correspond to neutrino (anti-neutrino) scattering using the iron PDFs from the 'A2' fit.

We have computed $R$ using both the Base-1 and Base-2 PDFs for the denominator of Eq. (2); recall that Base-1 includes a deuteron correction while Base-2 uses the CCFR data and does not include a deuteron correction. The difference between the Base-1 and Base-2 curves is approximately $2 \%$ at small $x$ and grows to $5 \%$ at larger $x$, with Base-2 above the Base- 1 results. The difference of these curves, in part, reflects the uncertainty introduced by the proton PDF [2]. As this behavior is typical, in the following plots (Figs. 4) we will only show the Base-1 results. We also observe that the neutrino (anti-neutrino) results coincide in the region of large $x$ where the valence


Figure 4. Nuclear correction factor $R$ for the structure function $F_{2}$ in neutrino and anti-neutrino scattering from Fe for $Q^{2}=\{5,20\} \mathrm{GeV}^{2}$. The solid curve shows the result of our analysis of NuTeV data; the uncertainty from the fit is represented by the shaded (yellow) band. For comparison we show the correction factor from the Kulagin-Petti model (dashed-dot line) [28], HKN07 (dashed-dotted line) [8], and the SLAC/NMC parametrization (dashed line).

PDFs are dominant, but differ by a few percent at small $x$ due to the differing strange and charm distributions.
4.3. $\mathbf{R}$ Factors for $F_{2}^{\nu}\left(x, Q^{2}\right)$ and $F_{2}^{\bar{\nu}}\left(x, Q^{2}\right)$

We now compute the nuclear correction factors for charged current neutrino-iron scattering. The results for $\nu-F e$ and those of $\bar{\nu}-F e$ are shown in Fig. 4. The numerator in Eq. 2 has been computed using the nuclear PDF from fit ' A 2 ', and for the denominator we have used the Base-1 PDFs. For comparison we also show the correction factor from the Kulagin-Petti model [28, 29] (dashed-dotted), and the SLAC/NMC curve (dashed) which has been obtained from an
$A$ and $Q^{2}$-independent parameterization of calcium and iron charged-lepton DIS data.

Due to the neutron excess in iron, both our curves and the KP curves differ when comparing scattering for neutrinos and anti-neutrinos; the SLAC/NMC parameterization is the same in both figures. For our results (solid lines), the difference between the neutrino and anti-neutrino results is relatively small, of order $3 \%$ at $x=0.6$. Conversely, for the KP model (dashed-dotted lines) the $\nu-\bar{\nu}$ difference reaches $10 \%$ at $x \sim 0.7$, and remains sizable at lower values of $x$.

To demonstrate the dependence of the $R$ factor on the kinematic variables, in Fig. 4 we have plotted the nuclear correction factor for two sep-
arate values of $Q^{2}$. Again, our curves and the KP model yield different results for different $Q^{2}$ values, in contrast to the SLAC/NMC parameterization.
Comparing the nuclear correction factors for the $F_{2}$ structure function with those obtained for the differential cross section (Fig. 3), we see these are quite different, particularly at small $x$. Again, this is because the cross section $d^{2} \sigma$ is comprised of a different combination of PDFs than the $F_{2}$ structure function. In general, our $R$-values for $F_{2}$ lie below those of the corresponding $R$-values for the cross section $d \sigma$ at small $x$. Since $d \sigma$ is a linear combination of $F_{2}$ and $F_{3}$, the $R$-values for $F_{3}$ (not shown) therefore lie above those of $F_{2}$ and $d \sigma$. Again, we emphasize that it is important to use an appropriate nuclear correction factor which is matched to the particular observable.

As we observed in the previous section, our results have general features in common with the KP model and the SLAC/NMC parameterization, but the magnitude of the effects and the $x$-region where they apply are quite different. Our results are noticeably flatter than the KP and SLAC/NMC curves, especially at moderate$x$ where the differences are significant. The general trend we see when examining these nuclear correction factors is that the anti-shadowing region is shifted to smaller $x$ values and any turnover at low $x$ is minimal given the PDF uncertainties. In general, these plots suggest that the size of the nuclear corrections extracted from the NuTeV data are smaller than those obtained from charged lepton scattering (SLAC/NMC) or from the set of data used in the KP model. We will investigate this difference further in the following section.

## 4.4. $F_{2}^{F e} / F_{2}^{D}$ from Iron PDFs

Since the SLAC/NMC parameterization was fit to $F_{2}^{F e} / F_{2}^{D}$ for charged-lepton DIS data, we can perform a more balanced comparison by using our iron PDFs to compute this same quantity. The results are shown in Fig. 5 where we have used our iron PDFs to compute $F_{2}^{F e}$, and the Base-1 and Base-2 PDFs to compute $F_{2}^{D}$.

As with the nuclear correction factor results


Figure 5. Predictions (solid and dashed line) for the structure function ratio $F_{2}^{F e} / F_{2}^{D}$ using the iron PDFs extracted from fits to NuTeV neutrino and anti-neutrino data. The SLAC/NMC parameterization is shown with the dot-dashed line. The structure function $F_{2}^{D}$ in the denominator has been computed using either the Base-2 (solid line) or the Base-1 (dashed line) PDFs.
of the previous section, we find our results have some gross features in common while on a more refined level the magnitude of the nuclear corrections extracted from the CC iron data differs from the charged lepton data. In particular, we note that the so-called "anti-shadowing" enhancement at $x \sim[0.06-0.3]$ is not reproduced by the charged current (anti-)neutrino data. Examining our results among all the various $R[\mathcal{O}]$ calculations, we generally find that any nuclear enhancement in the small $x$ region is reduced and shifted to a lower $x$ range as compared with the SLAC/NMC parameterization. Furthermore, in the limit of large $x$ ( $x \gtrsim 0.6$ ) our results are slightly higher than the data, including the very precise SLAC-E139 points; however, the large theoretical uncertainties on $F_{2}^{D}$ in this $x$-region make it difficult to extract firm conclusions.
This discussion raises the more general question as to whether the charged current ( $\nu-F e$ ) and neutral current ( $\ell^{ \pm}-F e$ ) correction factors are entirely compatible $[15,34,35,36,37,38]$. There is a priori no requirement that these be equal; in fact, given that the $\nu-F e$ process in-
volves the exchange of a $W$ and the $\ell^{ \pm}-F e$ process involves the exchange of a $\gamma$ we necessarily expect this will lead to differences at some level. ${ }^{11}$

### 4.5. Future Studies

It is important to resolve whether the differences we observe in Fig. 5 arise from the uncertainty of the nuclear corrections, or if they are genuinely a consequence of $\mathrm{NC} / \mathrm{CC}$ effects. A combined analysis of CC neutrino and NC charged-lepton data sets will shed more light on these issues. To best address these questions, we need to include the nuclear dimension (parameterized by the nuclear A value) as a dynamic component of the global fit; this will allow us to fit both the CC $W^{ \pm}$-exchange processes at large A, as well as the the NC $\gamma$-exchange processes at small A in a coherent framework. Figure 6 presents an an illustrative example of how the PDFs can be extended to incorporate the necessary A dependence to implement such a program. This extended analysis with additional data sets is in progress, and should help clarify these questions.


Figure 6. Illustration of the gluon $\operatorname{PDF} x f_{g}^{A}(x, \mu)$ vs. $x$ as a function of the nuclear $A$. At small $x$ the lower curves correspond to larger A values.

[^89]
## 5. CONCLUSIONS

While the nuclear corrections extracted from charged current $\nu-F e$ scattering have similar characteristics as the neutral current $l^{ \pm}-F e$ charged-lepton results, the detailed $x$ and $Q^{2}$ behavior is quite different. This observation raises the deeper question as to whether the charged current and neutral current nuclear correction factors may be substantially different. This present study of the iron PDFs provides a foundation for a general investigation (involving a variable A parameter) that can definitively address this topic. Resolving these questions is essential if we are to reliably use the plethora of nuclear data to obtaining free-proton PDFs which form the basis of the LHC analyses.

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# Parton distribution function nuclear corrections for charged lepton and neutrino deep inelastic scattering processes 

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#### Abstract

We perform a $\chi^{2}$ analysis of nuclear parton distribution functions (NPDFs) using neutral current charged-lepton ( $\ell^{ \pm} A$ ) deeply inelastic scattering (DIS), and Drell-Yan data for several nuclear targets. The nuclear $A$ dependence of the NPDFs is extracted in a next-to-leading order fit. We compare the nuclear corrections factors $\left(F_{2}^{F e} / F_{2}^{D}\right)$ for this charged-lepton data with other results from the literature. In particular, we compare and contrast fits based upon the charged-lepton DIS data with those using neutrino-nucleon DIS data.


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## I. INTRODUCTION

## A. PDFs and nuclear corrections

Parton distribution functions (PDFs) are of supreme importance in contemporary high-energy physics as they are needed for the computation of reactions involving hadrons based on QCD factorization theorems [1-3]. For this reason various groups present global analyses of PDFs for protons [4-14] and nuclei [15-20] which are regularly updated in order to meet the increasing demand for precision. The PDFs are nonperturbative objects which must be determined by experimental input. To fully constrain the $x$ dependence and flavor dependence of the PDFs requires large data sets from different processes which typically include deeply inelastic scattering (DIS), Drell-Yan (DY), and jet production.

While some of this data is extracted from free protons, much is taken from a variety of nuclear targets. Because the neutrino cross section is so small, to obtain sufficient statistics for the neutrino-nuclear DIS processes it is necessary to use massive targets (e.g., iron, lead, etc.). Therefore, nuclear corrections are required if we are to include the heavy-target data into the global analysis of proton PDFs.

The heavy-target neutrino DIS data plays an important role in extracting the separate flavor components of the PDFs. In particular, this data set gives the most precise

[^90]PACS numbers: $12.38 .-\mathrm{t}$, 13.15.+g, 13.60. $-\mathrm{r}, 24.85 .+\mathrm{p}$
information on the strange quark PDF. As the strange quark uncertainty may limit the precision of particular Large Hadron Collider (LHC) $W$ and $Z$ measurements, the nuclear corrections and their uncertainties will have a broad impact on a comprehensive understanding of current and future data sets.

## B. Nuclear corrections in the literature

In previous PDF analyses [21,22], a fixed nuclear correction was applied to "convert" the data from a heavy target to a proton. As such, these nuclear correction factors were frozen at a fixed value. They did not adjust for the $Q^{2}$ scale or the physical observable $\left(F_{2}, F_{3}, \frac{d \sigma}{d x d y}\right)$, and they did not enter the PDF uncertainty analysis.

While this approach may have been acceptable in the past given the large uncertainties, improvements in both


FIG. 1. Nuclear correction ratio, $F_{2}^{F e} / F_{2}^{D}$, as a function of $x$. The parametrized curve is compared to SLAC and BCDMS data [23-29].
data and theory precision demand comparable improvements in the treatment of the nuclear corrections.

Figure 1 displays the $F_{2}^{F e} / F_{2}^{D}$ structure function ratio as measured by the SLAC and BCDMS collaborations. The SLAC/NMC curve is the result of an $A$-independent parametrization fit to calcium and iron charged-lepton DIS data [23-30]. This parametrization was used to convert heavy-target data to proton data, which then would be input into the global proton PDF fit. ${ }^{1}$ The SLAC/NMC parametrization was then applied to both charged-leptonnucleus and neutrino-nucleus data, and this correction was taken to be independent of the scale $Q$ and the specific observable $\left\{F_{2}, F_{3}, \ldots\right\}$. Recent work demonstrates that the parametrized approximation of Fig. 1 is not sufficient and it is necessary to account for these details [31-33].

## C. Outline

In this paper, we present a new framework for a global analysis of nuclear PDFs (NPDFs) at next-to-leading order (NLO). An important and appealing feature of this framework is that it naturally extends the proton analysis by endowing the free fit parameters with a dependence on the atomic number $A$. This will allow us to study proton and nuclear PDFs simultaneously such that nuclear correction factors needed for the proton analysis can be computed dynamically.

In Sec. II, we outline our method for the analysis, specify the DIS and DY data sets, and present the $\chi^{2}$ of our fit. In Sec. III, we compute the nuclear correction factors $\left(F_{2}^{F e} / F_{2}^{D}\right)$ for the fit to the $\ell^{ \pm} A$ and DY data. In Sec. IV, we compare these results to the nuclear correction factors $\left(F_{2}^{F e} / F_{2}^{D}\right)$ from the $\nu A$ fit of Ref. [33]. Finally, we summarize our results in Sec. V.

## II. NPDF GLOBAL ANALYSIS FRAMEWORK

## A. PDF analysis framework

In this section, we present the global analysis of NPDFs using charged-lepton DIS ( $l^{ \pm} A$ ) and Drell-Yan data to extend the analysis of Ref. [30] for a variety of nuclear targets. This analysis is performed in close analogy with what is done for the $A=1$ free proton case [34]. We will use the general features of the QCD-improved parton model and the $\chi^{2}$ analyses as outlined in Ref. [33]. The input distributions are parametrized as

$$
\begin{aligned}
x f_{k}\left(x, Q_{0}\right) & =c_{0} x^{c_{1}}(1-x)^{c_{2}} e^{c_{3} x}\left(1+e^{c_{4}} x\right)^{c_{5}} \\
k & =u_{v}, d_{v}, g, \bar{u}+\bar{d}, s, \bar{s}
\end{aligned}
$$

$\bar{d}\left(x, Q_{0}\right) / \bar{u}\left(x, Q_{0}\right)=c_{0} x^{c_{1}}(1-x)^{c_{2}}+\left(1+c_{3} x\right)(1-x)^{c_{4}}$,

[^91]at the scale $Q_{0}=1.3 \mathrm{GeV}$. Here, the $u_{v}$ and $d_{v}$ are the upand down-quark valence distributions, $\bar{u}, \bar{d}, s, \bar{s}$ are the antiup, antidown, strange, and antistrange sea distributions, and $g$ is the gluon.

We note that there is a new series of PDFs in the literature from the NNPDF Collaboration [4,5,12-14] which are generated using a neural network. This approach has the advantage that no initial $x$-dependent parametrization is required. In comparison to the ansatz of Eq. (1), the neural network approach generally yields wider error bands, particularly in the small- $x$ region. This reflects, in part, the fact that the small- $x$ region is dominantly controlled by the $c_{1}$ parameter of Eq. (1), and this parameter is constrained by data at moderate to small values of $x$. With sufficiently precise data the errors given, for example, by the Hessian technique, may well be small, leading to relatively small errors for the extrapolation of the PDFs outside the region where the fits were constrained by data. In such cases, the parametrization-independent NNPDF estimates may well be more realistic, as they express the larger uncertainties in regions not directly constrained by data.

In order to accommodate different nuclear target materials, we introduce a nuclear $A$ dependence in the $c_{k}$ coefficients:
$c_{k} \rightarrow c_{k}(A) \equiv c_{k, 0}+c_{k, 1}\left(1-A^{-c_{k, 2}}\right), \quad k=\{1, \ldots, 5\}$.

This ansatz has the advantage that in the limit $A \rightarrow 1$ we have $c_{k}(A) \rightarrow c_{k, 0}$; hence, $c_{k, 0}$ is simply the corresponding coefficient of the free proton. Thus, we can relate the $c_{k, 0}$ parameters to the analogous quantities from proton PDF studies.

It is noteworthy that the $x$ dependence of our input distributions $f_{k}^{p / A}\left(x, Q_{0}\right)$ is the same for all nuclei $A$; hence, this approach treats the NPDFs and the proton PDFs on the same footing. ${ }^{2}$ Additionally, this method facilitates the interpretation of the fit at the parameter level by allowing us to study the $c_{k}(A)$ coefficients as functions of the nuclear A parameter.

With the $A$-generalized set of initial PDFs, we can apply the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) evolution equations to obtain the PDFs for a bound proton inside a nucleus $A, f_{i}^{p / A}(x, Q)$. We can then construct the PDFs for a general $(A, Z)$ nucleus:

$$
\begin{equation*}
f_{i}^{(A, Z)}(x, Q)=\frac{Z}{A} f_{i}^{p / A}(x, Q)+\frac{(A-Z)}{A} f_{i}^{n / A}(x, Q) \tag{3}
\end{equation*}
$$

where we relate the distributions of a bound neutron, $f_{i}^{n / A}(x, Q)$, to those of a proton by isospin symmetry.

[^92]Similarly, the nuclear structure functions are given by

$$
\begin{equation*}
F_{i}^{(A, Z)}(x, Q)=\frac{Z}{A} F_{i}^{p / A}(x, Q)+\frac{(A-Z)}{A} F_{i}^{n / A}(x, Q) . \tag{4}
\end{equation*}
$$

These structure functions can be computed at next-toleading order as convolutions of the nuclear PDFs with the conventional Wilson coefficients, i.e., generically

$$
\begin{equation*}
F_{i}^{(A, Z)}(x, Q)=\sum_{k} C_{i k} \otimes f_{k}^{(A, Z)} . \tag{5}
\end{equation*}
$$

To account for heavy quark mass effects, we calculate the relevant structure functions in the Aivazis-Collins-OlnessTung (ACOT) scheme [35,36] at NLO QCD [37].

TABLE I. The DIS $F_{2}^{A} / F_{2}^{D}$ data sets used in the fit. The table details the specific nuclear targets, references, and the number of data points without kinematical cuts.

| $F_{2}^{A} / F_{2}^{D}:$ |  |  | Number of <br> Observable |
| :--- | :---: | :---: | :---: |
| D | Experiment | Reference | data points |

TABLE II. The DIS $F_{2}^{A} / F_{2}^{A^{\prime}}$ data sets used in the fit. The table details the specific nuclear targets, references, and the number of data points without kinematical cuts.

| $F_{2}^{A} / F_{2}^{A^{\prime}}:$ |  |  | Number of <br> Observable |
| :--- | :---: | :---: | :---: |
| $\mathrm{Be} / \mathrm{C}$ | Experiment | Reference | data points |
| $\mathrm{Al} / \mathrm{C}$ | NMC-96 | $[48]$ | 15 |
| $\mathrm{Ca} / \mathrm{C}$ | NMC-96 | $[48]$ | 15 |
|  | NMC-95 | $[39]$ | 20 |
| $\mathrm{Fe} / \mathrm{C}$ | NMC-96 | $[48]$ | 15 |
| $\mathrm{Sn} / \mathrm{C}$ | NMC-95 | $[48]$ | 15 |
| $\mathrm{~Pb} / \mathrm{C}$ | NMC-96 | $[49]$ | 144 |
| $\mathrm{C} / \mathrm{Li}$ | NMC-96 | $[48]$ | 15 |
| $\mathrm{Ca} / \mathrm{Li}$ | NMC-95 | $[39]$ | 20 |
| $\mathrm{Total}:$ | NMC-95 | $[39]$ | 20 |

TABLE III. The Drell-Yan data sets used in the fit. The table details the specific nuclear targets, references, and the number of data points without kinematical cuts.

| $\sigma_{D Y}^{p A} / \sigma_{D Y}^{p A^{\prime}}:$ <br> Observable | Experiment | Reference | Number of <br> data points |
| :--- | :---: | :---: | :---: |
| $\mathrm{C} / \mathrm{D}$ | FNAL-E772-90 | $[50]$ | 9 |
| $\mathrm{Ca} / \mathrm{D}$ | FNAL-E772-90 | $[50]$ | 9 |
| $\mathrm{Fe} / \mathrm{D}$ | FNAL-E772-90 | $[50]$ | 9 |
| $\mathrm{~W} / \mathrm{D}$ | FNAL-E772-90 | $[50]$ | 9 |
| $\mathrm{Fe} / \mathrm{Be}$ | FNAL-E866-99 | $[51]$ | 28 |
| W/Be | FNAL-E866-99 | $[51]$ | 28 |
| Total: |  |  | 92 |

## B. Inputs to the global NPDF fit

Using the above framework, we can then construct a global fit to charged-lepton-nucleus ( $l^{ \pm} A$ ) DIS data and Drell-Yan data. To guide our constraints on the $c_{k, 0}$ coefficients, we use the global fit of the proton PDFs based upon Ref. [30]. This fit has the advantage that the extracted proton PDFs have minimal influence from nuclear targets. To provide the $A$-dependent nuclear information, we use a variety of $l^{ \pm} A$ DIS data and Drell-Yan data. The complete list of nuclear targets and processes is listed in Tables I, II, and III; there are 1233 data points before kinematical cuts are applied.

The structure of the fit is analogous to that of Ref. [33]. For the quark masses we take $m_{c}=1.3 \mathrm{GeV}$ and $m_{b}=$ 4.5 GeV . To limit effects of higher-twist we choose standard kinematic cuts of $Q_{\text {cut }}=2.0 \mathrm{GeV}$, and $W_{\text {cut }}=$ 3.5 GeV as they are employed in the CTEQ proton analyses. ${ }^{3}$ There are 708 data points which satisfy these cuts.

[^93]

FIG. 2 (color online). We display the $A$-dependent coefficients $c_{k}(A), k=\{1,5\}$, for the up-valence (top) and down-valence PDF (bottom) as a function of the nuclear $A$. The dependence of the coefficients $c_{k}(A)$ is shown by the following lines: $c_{1}$ solid (red) line, $c_{2}$ long-dashed (blue) line, $c_{3}$ dashed (green) line, $c_{4}$ dash-dotted (magenta) line, and $c_{5}$ dotted (brown) line.


FIG. 3 (color online). We display the (a) $x u(x)$ and (b) $x d(x)$ PDFs for a selection of nuclear $A$ values ranging from $A=\{1,207\}$. We choose $Q_{0}=1.3 \mathrm{GeV}$. The different curves depict the PDFs of nuclei with the following atomic numbers (from top to bottom at $x=0.01) A=1,2,4,8,20,54$, and 207.



FIG. 4 (color online). The computed nuclear correction ratio, $F_{2}^{F e} / F_{2}^{D}$, as a function of $x$ for $Q^{2}=5 \mathrm{GeV}^{2}$. (a) shows the fit (fit B) using charged-lepton-nucleus ( $\ell^{ \pm} A$ ) and DY data whereas (b) shows the fit using neutrino-nucleus ( $\nu A$ ) data (fit A2 from Ref. [33]). Both fits are compared with the SLAC/NMC parametrization, as well as fits from Kulagin-Petti (KP) (Ref. [31,32]) and Hirai et al. (HKN07), (Ref. [15]). The data points displayed in (a) are the same as in Fig. 1 and those displayed in (b) come from the NuTeV experiment [53,54].

## A. Charged-lepton $\left(\ell^{ \pm} A\right)$ data

The present nuclear PDF global analysis provides us with a complete set of NPDFs $f_{i}^{A}(x, Q)$ with full functional dependence on $\{x, Q, A\}$. Consequently, the traditional nuclear correction $F_{2}^{F e} / F_{2}^{D}$ does not have to be applied as a "frozen" external factor, but can now become a dynamic part of the fit which can be adjusted to accommodate the various data sets.

Having performed the fit outlined in Sec. II, we can then use the $f_{i}^{A}(x, Q)$ to construct the corresponding quantity $F_{2}^{F e} / F_{2}^{D}$ to find the form that is preferred by the data. In order to construct the ratio, we use the expression given by Eq. (4) for iron and deuterium. This result is displayed in Fig. 4(a) for a scale of $Q^{2}=5 \mathrm{GeV}^{2}$, and in Fig. 5(a) for a scale of $Q^{2}=20 \mathrm{GeV}^{2}$. Comparing these figures, we immediately note that our ratio $F_{2}^{\mathrm{Fe}} / F_{2}^{D}$ has nontrivial $Q$ dependence-as it should.

Figures 4(a) and 5(a) also compare our extracted $F_{2}^{F e} / F_{2}^{D}$ ratio with the ( $Q$-independent) SLAC/NMC parametrization of Fig. 1 and with the fits from Kulagin-Petti (KP) $[31,32]$. We observe that in the intermediate range ( $x \in \sim[0.07,0.7]$ ) where the bulk of the SLAC/NMC data constrains the parametrization, our computed $F_{2}^{F e} / F_{2}^{D}$ ratio compares favorably. When comparing the different curves, one has to bear in mind the following two points. First, all curves in principle have an uncertainty band which is not shown. Second, the data points used to extract the SLAC/NMC curve are measured at different $Q^{2}$ whereas our curve is always at a fixed $Q^{2}=5 \mathrm{GeV}^{2}$ or $Q^{2}=20 \mathrm{GeV}^{2}$. In light of these facts, we conclude that our fit agrees very well with other models and parametrizations as well as with the measured data points.

It should be noted that the kinematic cuts we employed to avoid higher twist effects effectively exclude all data


FIG. 5 (color online). Same as Fig. 4 for $Q^{2}=20 \mathrm{GeV}^{2}$.
points in the high- $x$ region above $x \gtrsim 0.7$. This is reflected by the fact that our curves in Figs. 4(a) and 5(a) stop at $x=$ 0.7 . The high- $x$ region is beyond the scope of this paper and will be the subject of a future analysis.

Thus, we find that data sets used in this fit $\left(F_{2}^{A} / F_{2}^{D}\right.$, $F_{2}^{A} / F_{2}^{A^{\prime}}$, and $\sigma_{D Y}^{p A} / \sigma_{D Y}^{p A^{\prime}}$ ) are compatible with the SLAC, BCDMS, and NMC data. Additionally, we can go further and use our complete set of NPDFs $f_{i}^{A}(x, Q)$ to compute the appropriate nuclear correction not only for $F_{2}^{F e} / F_{2}^{D}$, but for any nuclear target $(A)$ for any $Q$ value, and for any observable. We make use of this property in the following section where we compute the corresponding quantity for a different nuclear process.

## IV. $\ell^{ \pm} \boldsymbol{A}$ AND $\boldsymbol{\nu} \boldsymbol{A}$ NUCLEAR CORRECTIONS

## A. Nuclear corrections in $\boldsymbol{\nu} \boldsymbol{A}$ DIS

In a previous analysis [33], we examined the charged current (CC) neutrino-nucleus DIS process $\nu A \rightarrow \mu X$, and extracted the $F_{2}^{F e} / F_{2}^{D}$ ratio. ${ }^{4}$

These results are displayed in Figs. 4(b) and 5(b). The solid line is the result of the global fit (fit A2), and this is compared with the previous SLAC/NMC parametrization, as well as fits KP and HKN07. The data points displayed come from the NuTeV experiment [53,54]. The (yellow) band is an approximation of the uncertainty of the fits.

As observed above, the SLAC/NMC parametrization is generally consistent with the results of KP and HKN as well as our B fit to $\ell^{ \pm} A$ and DY data. However, the A2 fit of Figs. 4(b) and 5(b) does not agree with any of these three results. We now examine this in detail.

## B. $\ell^{ \pm} A$ and $\nu \boldsymbol{A}$ comparison

The contrast between the charged-lepton $\left(\ell^{ \pm} A\right)$ case and the neutrino $(\nu A)$ case is striking; while the charged-lepton results generally align with the SLAC/NMC, KP, and HKN determinations, the neutrino results clearly yield different behavior in the intermediate $x$ region. We emphasize that both the charged-lepton and neutrino results are not a model-they come directly from global fits to the data. To emphasize this point, we have superimposed illustrative data points in Figs. 4(b) and 5(b); these are simply the $\nu A$ DIS data $[53,54]$ scaled by the appropriate structure function, calculated with the proton PDF of Ref. [33].

The mismatch between the results in charged-lepton and neutrino DIS is particularly interesting given that there has been a long-standing "tension" between the light-target charged-lepton data and the heavy-target neutrino data in the historical fits $[55,56]$. This study demonstrates that the tension is not only between charged-lepton light-target

[^94]data and neutrino heavy-target data, but we now observe this phenomenon in comparisons between neutrino and charged-lepton heavy-target data.

There are two possible interpretations of this result.
(1) There is, in fact, a single "compromise" solution for the $F_{2}^{F e} / F_{2}^{D}$ nuclear correction factor which yields a good fit for both the $\nu A$ and $\ell^{ \pm} A$ data.
(2) The nuclear corrections for the $\ell^{ \pm} A$ and $\nu A$ processes are different.

Considering possibility 1 , the "apparent" discrepancy observed in Figs. 4 and 5 could simply reflect uncertainties in the extracted nuclear PDFs. The global fit framework introduced in this work paves the way for a unified analysis of the $\ell^{ \pm} A$, DY, and $\nu A$ data which will ultimately answer this question. Having established the nuclear correction factors for neutrino and charged-lepton processes separately, we can combine these data sets (accounting for appropriate systematic and statistical errors) to obtain a compromise solution. ${ }^{5}$

If it can be established that a compromise solution does not exist, then the remaining option is that the nuclear corrections in neutrino and charged-lepton DIS are different. This idea has previously been discussed in the literature [31,32,57]. We note that the charged-lepton processes occur (dominantly) via $\gamma$ exchange, while the neutrinonucleon processes occur via $W^{ \pm}$exchange. Thus, the different nuclear corrections could simply be a consequence of the differing propagation of the intermediate bosons (photon, $W$ ) through dense nuclear matter. Regardless of whether this dilemma is resolved via option 1 or 2, understanding this puzzle will provide important insights about processes involving nuclear targets. Furthermore, a deeper understanding could be obtained by a future high-statistics, high-energy neutrino experiment using several nuclear target materials [58-60].

## V. CONCLUSIONS

We presented a new framework to carry out a global analysis of NPDFs at next-to-leading order QCD, treating proton and nuclear targets on equal footing. Within this approach, we have performed a $\chi^{2}$ analysis of nuclear PDFs by extending the proton PDF fit of Ref. [30] to DIS $l^{ \pm} A$ and Drell-Yan data. The result of the fit is a set of nuclear PDFs which incorporate not only the $\{x, Q\}$ dependence, but also the nuclear- $A$ degree of freedom; thus we can accommodate the full range of nuclear targets from light $(A=1)$ to heavy $(A=207)$. We find a good fit to the

[^95]combined data set with a total $\chi^{2} /$ DOF of 0.946 demonstrating the viability of the framework.

We have used our results to compute the nuclear corrections factors, and to compare these with the results from the literature. We find good agreement for those fits based on a charged-lepton data set.

Separately, we have compared our nuclear corrections (derived with a charged-lepton data set) with those computed using neutrino DIS $(\nu A \rightarrow \mu X)$ data sets. Here, we observe substantive differences.

This fit is novel in several respects.
(i) Since we constructed the nuclear PDF fits analogous to the proton PDF fits, this framework allows a meaningful comparison between these two distributions.
(ii) The above unified framework integrates the nuclear correction factors as a dynamic component of the fit. These factors are essential if we want to use the heavy-target DIS data to constrain the strange quark distribution of the proton, for example.
(iii) This unified analysis of proton and nuclear PDFs provides the foundation necessary to simultaneously analyze $\ell^{ \pm} A$, DY, and $\nu A$ data. This will ultimately help in determining whether (1) a compromise solution exists, or (2) the nuclear corrections depend on the exchanged boson (e.g., $\gamma / Z$ or $\left.W^{ \pm}\right)$.
ing and important question. The resolution of this issue is essential for a complete understanding of both the proton and nuclear PDFs.

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# Nuclear Corrections in Neutrino-Nucleus Deep Inelastic Scattering and their Compatibility with Global Nuclear Parton-Distribution-Function Analyses 

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#### Abstract

We perform a global $\chi^{2}$ analysis of nuclear parton distribution functions using data from charged current neutrino-nucleus ( $\nu A$ ) deep-inelastic scattering (DIS), charged-lepton-nucleus ( $\ell^{ \pm} A$ ) DIS, and the Drell-Yan (DY) process. We show that the nuclear corrections in $\nu A$ DIS are not compatible with the predictions derived from $\ell^{ \pm} A$ DIS and DY data. We quantify this result using a hypothesis-testing criterion based on the $\chi^{2}$ distribution which we apply to the total $\chi^{2}$ as well as to the $\chi^{2}$ of the individual data sets. We find that it is not possible to accommodate the data from $\nu A$ and $\ell^{ \pm} A$ DIS by an acceptable combined fit. Our result has strong implications for the extraction of both nuclear and proton parton distribution functions using combined neutrino and charged-lepton data sets.


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High statistics neutrino deep-inelastic scattering (DIS) experiments have generated significant interest in the literature as they provide crucial information for global fits of parton distribution functions (PDFs). The neutrino DIS data provide the most stringent constraints on the strange quark distribution in the proton, and allow for flavor decomposition of the PDFs which is essential for precise predictions of the benchmark gauge boson production processes at the LHC. Moreover, the neutrino experiments have been used to make precision tests of the standard model (SM). A prominent example is the extraction of the weak mixing angle $\theta_{W}$ in a Paschos-Wolfenstein type analysis [1]. A good knowledge of the neutrino DIS cross sections is also very important for long baseline experiments of the next generation which aim at measuring small parameters of the mixing matrix such as the mixing angle $\theta_{13}$ and eventually the $C P$ violating phase $\delta$.

Because of the weak nature of neutrino interactions the use of heavy nuclear targets is unavoidable, and this complicates the analysis of the precision physics discussed above since model-dependent nuclear corrections must be applied to the data. Our present understanding of the nuclear corrections is mainly based on charged-leptonnucleus ( $\ell A$ ) DIS data. In the early 80s the European Muon Collaboration (EMC) [2] found that the nucleon structure functions $F_{2}$ for iron and deuterium differ. This discovery triggered a vast experimental program to investigate the nuclear modifications of the ratio $R\left[F_{2}^{\ell A}\right]=$ $F_{2}^{\ell A} /\left(A F_{2}^{\ell N}\right)$ for a wide range of nuclear targets with atomic number $A$, see Table I. By now, such modifications have been established in a kinematic range from relatively small

Bjorken $x\left(x \sim 10^{-2}\right)$ to large $x(x \sim 0.8)$ in the deepinelastic region with squared momentum transfer $Q^{2}>$ $1 \mathrm{GeV}^{2}$. The behavior of the ratio $R\left[F_{2}^{\ell A}\right]$ can be divided into four regions: (i) $R>1$ for $x \gtrsim 0.8$ (Fermi motion region), (ii) $R<1$ for $0.25 \leqq x \leqq 0.8$ (EMC region), (iii) $R>1$ for $0.1 \leqq x \leqq 0.25$ (antishadowing region), and (iv) $R<1$ for $x \leqq 0.1$ (shadowing region), with different physics mechanisms explaining the nuclear modifications. The shadowing suppression at small $x$ occurs due to coherent multiple scattering inside the nucleus of a $q \bar{q}$ pair coming from the virtual photon [5] with destructive interference of the amplitudes [6]. The antishadowing region is theoretically less well understood but might be explained by the same mechanism with constructive interference of the multiple scattering amplitudes [6] or by the application of momentum, charge, and/or baryon number sum rules. Conversely, the modifications at medium and large $x$ are usually explained by nuclear binding and medium effects and the Fermi motion of the nucleons [7].

Instead of trying to address the origin of the nuclear effects, the data on nuclear structure functions can be analyzed in terms of nuclear PDFs (NPDFs) which are modified as compared to the free nucleon PDFs. Relying on factorization theorems in the same spirit as in the free nucleon case, the advantage of this approach is that the universal NPDFs can be used to make predictions for a large variety of processes in $\ell A, \nu A, p A$, and $A A$ collisions. In addition, the nuclear correction factors required for the interpretation of the neutrino experiments can be calculated in a flexible way, taking into account the precise observable, the nuclear $A$, and the scale $Q^{2}$. The factorization assumption in the
nuclear environment is therefore a question of considerable theoretical and practical importance and global analyses of NPDFs based on $\ell A$ DIS and fixed target Drell-Yan (DY) data confirm its validity in the presently explored kinematic range.

However, in a recent analysis [3] of $\nu \mathrm{Fe}$ DIS data from the NuTeV collaboration we found that the nuclear correction factors are surprisingly different from the predictions based on the $\ell^{ \pm} \mathrm{Fe}$ charged-lepton results with important implications for global analyses of proton PDFs. This is not

TABLE I. The charged-lepton DIS data sets together with DY and with neutrino DIS data sets used in the fit. The table details the specific nuclear targets, and the number of data points with kinematical cuts ( $Q^{2}>4 \mathrm{GeV}^{2}, W>3.5 \mathrm{GeV}$ ). References for the data sets are cited in Refs. [3,4].

| ID | Observable | $A / A^{\prime}(A)$ | Experiment | \# data |
| :---: | :---: | :---: | :---: | :---: |
| 1 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{He} / \mathrm{D}$ | SLAC-E139, NMC-95,re | 15 |
| 2 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Li/D | NMC-95 | 11 |
| 3 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Be/D | SLAC-E139 | 3 |
| 4 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | C/D | EMC-88, 90, SLAC-E139, NMC-95,re, FNAL-E665-95 | 38 |
| 5 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | N/D | BCDMS-85 | 9 |
| 6 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Al/D | SLAC-E049 E139 | 3 |
| 7 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Ca} / \mathrm{D}$ | EMC-90, SLAC-E139, NMC-95,re, FNAL-E665-95 | 17 |
| 8 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Fe} / \mathrm{D}$ | BCDMS-85, 87, SLAC-E049, E139, E140 | 24 |
| 9 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Cu} / \mathrm{D}$ | EMC-88, 93 | 27 |
| 10 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Ag/D | SLAC-E139 | 2 |
| 11 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Sn/D | EMC-88 | 8 |
| 12 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Xe/D | FNAL-E665-92 | 2 |
| 13 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Au} / \mathrm{D}$ | SLAC-E139 | 3 |
| 14 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Pb} / \mathrm{D}$ | FNAL-E665-95 | 3 |
| 15 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Be} / \mathrm{C}$ | NMC-96 | 14 |
| 16 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Al/C | NMC-96 | 14 |
| 17 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Ca} / \mathrm{C}$ | NMC-95, 96 | 29 |
| 18 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Fe/C | NMC-95 | 14 |
| 19 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Pb} / \mathrm{C}$ | NMC-96 | 14 |
| 20 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{C} / \mathrm{Li}$ | NMC-95 | 7 |
| 21 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{Ca} / \mathrm{Li}$ | NMC-95 | 7 |
| 22 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | $\mathrm{He} / \mathrm{D}$ | Hermes | 17 |
| 23 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Kr/D | Hermes | 12 |
| 24 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | Sn/C | NMC-96 | 111 |
| 25 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | N/D | Hermes | 19 |
| 32 | $F_{2}^{A} / F_{2}^{A^{\prime}}$ | D | NMC-97 | 201 |
| 26 | $\sigma_{\mathrm{DY}}^{p A} / \sigma_{\mathrm{DY}}^{p A^{\prime}}$ | C/D | FNAL-E772 | 9 |
| 27 | $\sigma_{\mathrm{DY}}^{p A} / \sigma_{\mathrm{DY}}^{P A^{\prime}}$ | $\mathrm{Ca} / \mathrm{D}$ | FNAL-E772 | 9 |
| 28 | $\sigma_{\mathrm{DY}}^{p A} / \sigma_{\mathrm{DY}}^{p A^{\prime}}$ | Fe/D | FNAL-E772 | 9 |
| 29 | $\sigma_{\mathrm{DY}}^{p A} / \sigma_{\mathrm{DY}}^{p A^{\prime}}$ | W/D | FNAL-E772 | 9 |
| 30 | $\sigma_{\mathrm{DY}}^{p A} / \sigma_{\mathrm{DY}}^{p A^{\prime}}$ | $\mathrm{Fe} / \mathrm{Be}$ | FNAL-E866 | 28 |
| 31 | $\sigma_{\text {DY }}^{p A} / \sigma_{\mathrm{DY}}^{p A^{\prime}}$ | W/Be | FNAL-E866 | 28 |
|  |  |  | $l^{ \pm} A$ DIS \& DY Total: | 708 |
| 33 | $d \sigma^{\nu A} / d x d y$ | Pb | CHORUS $\nu$ | 824 |
| 34 | $d \sigma^{\nu A} / d x d y$ | Pb | CHORUS $\bar{\nu}$ | 412 |
| 35 | $d \sigma^{\nu A} / d x d y$ | Fe | NuTeV $\nu$ | 1170 |
| 36 | $d \sigma^{\nu A} / d x d y$ | Fe | NuTeV $\bar{\nu}$ | 966 |
| 37 | $d \sigma^{\nu A} / d x d y$ | Fe | CCFR di- $\mu$ | 44 |
| 38 | $d \sigma^{\nu A} / d x d y$ | Fe | NuTeV di- $\mu$ | 44 |
| 39 | $d \sigma^{\nu A} / d x d y$ | Fe | CCFR di- $\mu$ | 44 |
| 40 | $d \sigma^{\nu A} / d x d y$ | Fe | NuTeV di- $\mu$ | 42 |
|  |  |  | $\nu A$ Total: | 3134 |

completely unexpected since the structure functions in charged current (CC) neutrino DIS and neutral current (NC) electron or muon DIS are distinct observables with different parton model expressions. From this perspective it is clear that the nuclear correction factors will not be exactly the same even for a universal set of NPDFs. Note also that some models in the literature predict differences between reactions in CC and NC DIS [8]. What is, however, unexpected is the degree to which the $R$ factors differ between the structure functions $F_{2}^{\nu \mathrm{Fe}}$ and $F_{2}^{\ell \mathrm{Fe}}$. In particular the lack of evidence for shadowing in neutrino scattering down to $x \sim 0.02$ is quite surprising.

The study in Ref. [3] left open the question, whether the neutrino DIS data could be reconciled with the chargedlepton DIS data by a better flavor separation of the NPDFs. In this letter, we address this question in the $A$-dependent framework of Ref. [4] by performing a global $\chi^{2}$ analysis of the combined data from $\nu A$ DIS, $\ell A$ DIS and the DY process listed in Table I.

When combining neutrino and charged-lepton + DY data into a compromise fit, we introduce a weight parameter $w$ into the $\chi^{2}$ via

$$
\begin{equation*}
\chi^{2}=\sum_{l^{ \pm} A \text { data }} \chi_{i}^{2}+\sum_{\nu A \text { data }} w \chi_{i}^{2} \tag{1}
\end{equation*}
$$

The $w$ factor allows us to adjust for the different number of points in the separate data sets, and provides a parameter that interpolates between the $\nu A$ and the $\ell^{ \pm} A+\mathrm{DY}$ data. We should stress that the $\chi^{2}$ cited in Table II and also in the text is the standard $\chi^{2}$; Eq. (1) is only used internally in the fitting procedure. We construct a set of compromise fits with weights $w=\left\{0, \frac{1}{7}, \frac{1}{2}, 1, \infty\right\}$ and study the dependence of the result on this weight. The fit to only neutrino data, denoted $w=\infty$ in Table II, is compatible with the results in [3]. Similarly, the fit to only charged-lepton + DY data, denoted $w=0$, agrees well with the analysis in [4].

We first compute the nuclear correction factors $R\left[F_{2}^{\ell \mathrm{Fe}}\right] \simeq F_{2}^{\ell \mathrm{Fe}} / F_{2}^{\ell N}$ and $R\left[F_{2}^{\nu \mathrm{Fe}}\right] \simeq F_{2}^{\nu \mathrm{Fe}} / F_{2}^{\nu N}$ in the QCD parton model at next-to-leading order employing the NPDF fits in Table II for the numerator and free nucleon PDFs for the denominator [9]. The $x$ dependence of $R\left[F_{2}^{\ell \mathrm{Fe}}\right]$ and $R\left[F_{2}^{\nu \mathrm{Fe}}\right]$ is shown in Figs. 1(a) and 1(b), respectively, at $Q^{2}=5 \mathrm{GeV}^{2}$. Similar results hold at $Q^{2}=20 \mathrm{GeV}^{2}$ which we do not present here. We observe that the fit to only $\ell A$ DIS + DY data $(w=0)$ well describes the SLAC and BCDMS points in Fig. 1(a). The same is true for the fit to only $\nu A$ DIS data $(w=\infty)$ which is compatible with the results from the NuTeV experiment

TABLE II. Summary table of a family of compromise fits.

| $w$ | $l^{ \pm} A$ | $\chi^{2}(/ \mathrm{pt})$ | $\nu A$ | $\chi^{2}(/ \mathrm{pt})$ | total $\chi^{2}(/ \mathrm{pt})$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| 0 | 708 | $638(0.90)$ | $\cdots$ | $\cdots$ | $638(0.90)$ |
| $1 / 7$ | 708 | $645(0.91)$ | 3134 | $4710(1.50)$ | $5355(1.39)$ |
| $1 / 2$ | 708 | $680(0.96)$ | 3134 | $4405(1.40)$ | $5085(1.32)$ |
| 1 | 708 | $736(1.04)$ | 3134 | $4277(1.36)$ | $5014(1.30)$ |
| $\infty$ | $\cdots$ | $\cdots$ | 3134 | $4192(1.33)$ | $4192(1.33)$ |

[10] exemplified in Fig. 1(b). However, comparing the results obtained with the $w=0$ and the $w=\infty$ fits one can see that they predict considerably different $x$ shapes.

The fits with weights $w=\left\{\frac{1}{7}, \frac{1}{2}, 1\right\}$ interpolate between these two incompatible solutions. As can be seen in Figs. 1(a) and 1(b), with increasing weight the description of the $\ell \mathrm{Fe}$ data is worsened in favor of a better agreement with the $\nu \mathrm{Fe}$ points. This trend clearly demonstrates that the $\ell \mathrm{Fe}$ and the $\nu \mathrm{Fe}$ data pull in opposite directions. We identify the fits with $w=1 / 2$ or $w=1$ as the best candidates for a possible compromise.

To be able to decisively accept or reject the compromise fits, we apply a statistical goodness-of-fit criterion [11-13] based on the probability distribution for the $\chi^{2}$ given that the fit has $N$ degrees of freedom:

$$
\begin{equation*}
P\left(\chi^{2}, N\right)=\frac{\left(\chi^{2}\right)^{N / 2-1} e^{-\chi^{2} / 2}}{2^{N / 2} \Gamma(N / 2)} \tag{2}
\end{equation*}
$$

This allows us to define the percentiles $\xi_{p}$ via $\int_{0}^{\xi_{p}} P\left(\chi^{2}, N\right) d \chi^{2}=p \% \quad$ where $\quad p=\{50,90,99\}$. Here, $\xi_{50}$ serves as an estimate of the mean of the $\chi^{2}$ distribution and $\xi_{90}$, for example, gives us the value where there is only a $10 \%$ probability that a fit with $\chi^{2}>\xi_{90}$ genuinely describes the given set of data. In a global PDF fit, the best fit $\chi^{2}$ value often deviates from the mean value because the data come from different possibly incompatible experiments having unidentified, unknown errors which are not accounted for in the experimental systematic errors. For this reason we rescale the $\xi_{90}$ and $\xi_{99}$ percen-


FIG. 1 (color online). Predictions from the compromise fits for the nuclear correction factors $R\left[F_{2}^{\ell \mathrm{Fe}}\right] \simeq F_{2}^{\ell \mathrm{Fe}} / F_{2}^{\ell N}$ (a) and $R\left[F_{2}^{\nu \mathrm{Fe}}\right] \simeq F_{2}^{\nu \mathrm{Fe}} / F_{2}^{\nu N}$ (b) as a function of $x$ for $Q^{2}=5 \mathrm{GeV}^{2}$. The data points displayed in (a) are from BCDMS and SLAC experiments (for references see [4]) and those displayed in (b) come from the NuTeV experiment [10].
tiles relative to the best fit $\chi_{0}^{2}$ [11] to define $C_{90}=$ $\chi_{0}^{2}\left(\xi_{90} / \xi_{50}\right)$ and $C_{99}=\chi_{0}^{2}\left(\xi_{99} / \xi_{50}\right)$. This defines our criterion: a fit with a given $\chi^{2}$ is compatible with the best fit with $\chi_{0}^{2}$ at $90 \%$ (99\%) confidence if $\chi^{2}<C_{90}$ ( $\chi^{2}<C_{99}$ ). We apply it to both the total $\chi^{2}$ and the $\chi^{2}$ of the individual data sets.

For the $\ell A$ DIS + DY data we use the fit with $w=0$ as benchmark with $\chi_{0}^{2}=638$ and $N=677$ degrees of freedom (for 708 data points and 31 free parameters). The upper limits on the $\chi^{2}$ at $90 \%$ and $99 \%$ confidence level (C.L.) are then $C_{90}^{I^{ \pm} A}=684$ and $C_{99}^{l^{ \pm} A}=722$. The benchmark fit for the $\nu A$ DIS data $(w=\infty)$ uses 3134 data points with 33 free parameters resulting in $N=3101$ and one finds $C_{90}^{\nu A}=4330$ and $C_{99}^{\nu A}=4445$. We see that none of the compromise fits satisfies both limits at the $90 \%$ C.L. which is usually used in global analyses of PDFs to define the uncertainty bands. At the $99 \%$ C.L., there are two fits $(w=1 / 2, w=1)$ which are below the $C_{99}^{\nu A}$ limit. However, only the $w=1 / 2$ fit satisfies the corresponding constraint from the charged-lepton benchmark fit.

We now apply our criterion also to the individual data sets with IDs between 1 and 40 in Table I. For the $\ell A$ DIS + DY data $(\mathrm{ID}=[1,31])$ we determine the $31 C_{90}$ ( $C_{99}$ ) limits by using the individual $\chi_{i}^{2}$ of the $w=0$ fit as $\chi_{0, i}^{2}$. For the $\nu A$ DIS data (ID $=[33,40]$ ) we proceed in a similar manner using the individual $\chi_{i}^{2}$ of the $w=\infty$ fit. The results of this detailed analysis are depicted in Fig. 2, where we show the quantity

$$
\begin{equation*}
\frac{\Delta \chi^{2}}{\Delta C_{90}}=\frac{\chi_{i}^{2}-\chi_{0, i}^{2}}{C_{90, i}-\chi_{0, i}^{2}} \quad(i=1, \ldots, 40), \tag{3}
\end{equation*}
$$

where $\chi_{i}^{2}$ represents the $\chi^{2}$-value of the $i$ th data set. In cases where $\chi_{i}^{2}>C_{90, i}$ the fit is not compatible with the best fit at the $90 \%$ level and $\Delta \chi^{2} / \Delta C_{90}>1$. The exact


FIG. 2 (color online). $\Delta \chi^{2} / \Delta C_{90}$ as defined in Eq. (3) for the 40 individual data sets. Results are shown for the $w=\frac{1}{2}$-fit (a) and the fit "Ucor5" (b) with $w=1$. The solid and dashed lines indicate the $90 \%$ and $99 \%$ confidence limits. The highlighted data sets correspond to DIS $\ell^{ \pm} \mathrm{Fe}(\mathrm{ID}=8), \nu \mathrm{Fe}(\mathrm{ID}=35)$, and $\bar{\nu} \mathrm{Fe}(\mathrm{ID}=36)$.
$90 \%$ C.L. limit is shown as a constant solid line and the dotted line represents the $99 \%$ confidence limit. The local application of the $\chi^{2}$ hypothesis-testing criterion reveals that even the compromise fit with weight $w=\frac{1}{2}$ which was considered acceptable at the $99 \%$ C.L. when looking at the nuclear correction factors and at the global change in $\chi^{2}$, cannot be accepted as a compromise solution as both the charged-lepton and neutrino DIS data on iron exceed the $99 \%$ limit.

In conclusion, the tension between the $\ell^{ \pm} \mathrm{Fe}$ and $\nu \mathrm{Fe}$ data sets leaves us with no possible compromise fit when investigating the results in detail, not even when using the $99 \%$ percentile as the limit as opposed to the more restrictive $90 \%$ limit which is usually used to construct the error PDFs. This detailed analysis confirms the preliminary conclusions of Refs. [3,4] that there is no possible compromise fit which adequately describes the neutrino DIS data along with the charged-lepton data.

At face value, this conclusion differs from some results in the literature which argue the $\nu A$ and $\ell^{ \pm} A$ data are in accord [14]. Here, we believe an essential element in our analysis is the use of the correlated systematic errors of the $\nu A$ data. To highlight this point, we now repeat our analysis, but we combine the statistical and all systematic errors in quadrature (thereby neglecting the information contained in the correlation matrix) for $\nu A$ data for the $w=1$ fit with $Q^{2}>4 \mathrm{GeV}$ (as before); we denote this the "Ucor4" fit, and we obtain $\chi^{2} / p t$ of 1.14 for $\ell^{ \pm} A$ and 1.00 for $\nu A$. We also use a $Q^{2}>5 \mathrm{GeV}$ fit (denoted "Ucor5") to mimic the cuts of Ref. [14]; here we obtain $\chi^{2} / p t$ of 1.14 for $\ell^{ \pm} A$ and 0.96 for $\nu A$.

If we examine the total $\chi^{2}$ values, we find the $\chi^{2} / \operatorname{dof} \sim 1$, and might be tempted to conclude we are able to fit both the $\nu A$ and $\ell^{ \pm} A$ data simultaneously. However, if we look at individual data sets and apply our hypothesis-testing criteria, the picture is quite different. Figure 2(b) displays the results for the Ucor5 fit. The higher $Q^{2}$ cut of the Ucor5 fit removes some of the very precise NuTeV data at small- $x$, thus resulting in an improved $\chi^{2}$ compared to Ucor4. Nevertheless, many of the $\ell^{ \pm} A$ data sets (ID $=3,4,5$, $6,8)$ still lie outside the $99 \%$ C.L. percentile. Thus, we still conclude that there is no compromise fit for the $\nu A$ and $\ell^{ \pm} A$ data even if we relax the constraints by using uncorrelated errors.

Consequently, the nuclear correction factor for the neutrino DIS data are indeed incompatible with that of the charged-lepton DIS and DY data, and this result depends crucially on the use of the precision correlated errors of the neutrino data. This result has important implications for both nuclear and proton PDFs. If we do not know the appropriate nuclear correction to relate different nuclear targets, our ability to extract PDFs is limited. For example, the CTEQ6.6 analysis [15] sidesteps these issues by removing most of the $\nu$ A data from the fit; however, they
retain the NuTeV dimuon data since this data is critical to constraining the strange quark PDF. This underscores the importance of the $\nu A$ data for flavor differentiation.

Although the NuTeV data provide the tightest constraints due to their statistics, we note that this issue cannot be tied to a single data set. For example, we find that NuTeV is generally compatible with CCFR and CDHSW [16]. The CHORUS $\nu P b$ and $\bar{\nu} P b$ data have larger uncertainties, so they can be compatible with both the $\ell^{ \pm} A$ data and the $\mathrm{NuTeV} \nu \mathrm{Fe}$ data because the $\Delta \chi^{2} / \Delta C_{90}<1$ for all weights. Compared to the theory predictions, NuTeV agrees well in the central $x$ region, but exhibits differences both for low $x$ at low $Q^{2}$, and also for very high $x(x \sim 0.65)$.

We have demonstrated that the $\nu A$ and $\ell^{ \pm} A$ data prefer different nuclear correction factors, and that there is no single "compromise" result that will simultaneously satisfy both data sets. While we have focused on the phenomenological aspects for the present study, this result has strong implications for the extraction of both nuclear and proton PDFs using combined neutrino and chargedlepton data sets. Possibilities include unexpectedly large higher-twist effects, or even nonuniversal nuclear effects; we leave such questions for a future study.
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# A Survey of Heavy Quark Theory for PDF Analyses 

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#### Abstract

We survey some of the recent developments in the extraction and application of heavy quark Parton Distribution Functions (PDFs). We also highlight some of the key HERA measurements which have contributed to these advances.


Keywords: Quantum Chromodynamics, Parton Distribution Functions, Heavy Quarks, Deeply Inelastic Scattering.

## Two Decades of HERA physics

The HERA electron-proton collider ring began its physics program in 1992 and completed accelerator operations in 2007. The data collected by the HERA facility allowed for physics studies over a tremendously expanded kinematic region compared to the previous fixed-target experiments. This point is illustrated in Figure 1 where we display the $e^{+} p$ Neutral Current (NC) cross section vs. $Q^{2}$ for the HERA data (runs I and II) together with the fixed-target data. We observe that the HERA data allows us to extend our reach in $Q^{2}$ by more than two decades for large to intermediate $x$ values, and also extends the small $x$ region down to $\sim 10^{-5}$.

Additionally, the large statistics and reduced systematics of the experimental data demand that the theoretical predictions keep pace. Over the lifetime of HERA we have seen many of the theoretical calculations advanced from Leading-Order (LO), to Next-to-Leading-Order (NLO), and some even to Next-to-Next-to-Leading-Order (NNLO).

As the required theoretical precision has increased, it has been necessary to revisit the many inputs and assumptions which are used in the calculations. We will


Figure 1: $e^{+} p$ NC cross section for the combined HERA data as compared with the HERAPDF1.5 fit as a function of $Q^{2}$ for different values of $x$. (Figure from H1prelim-10-142 \& ZEUS-prel-10-018.)

[^96]

Figure 2: The computed nuclear correction ratio, $F_{2}^{F e} / F_{2}^{N}$, as a function of $x$ for $Q^{2}=5 \mathrm{GeV}^{2}$. Figure-a) shows the fit (fit B from Ref. [16]) using charged-lepton-nucleus $\left(\ell^{ \pm} A\right)$ and DY data whereas Figure-b) shows the fit using neutrino-nucleus ( $v A$ ) data (fit A2 from Ref. [2]). Both fits are compared with the SLAC/NMC parameterization [16], as well as fits from Kulagin-Petti (KP) (Ref. [3, 4]) and Hirai et al. (HKN07), (Ref. [5]). The data points displayed in Figure-a) come from a selection of SLAC and BCDMS data. [6, 7, 8, 9, 10, 11, 12].
examine the role that the heavy quarks-and their associated masses-play in these calculations, both for the evolution of the parton distribution functions (PDFs) and also the hard-scattering cross sections.

## Determining the Heavy Quark PDFs

HERA's reach to larger $Q^{2}$ and smaller $x$ values takes us to a new kinematic region where the heavy quarks $(s, c, b)$ play a more important role. For example, the strange and charm quark contributions to $F_{2}$ at small $x$ values can be $30 \%$ or more of the total inclusive result. To make high-precision predictions for the structure functions we must therefore be capable of reducing the uncertainty of these heavy quark contributions; this requires, in part, precise knowledge of the PDFs which enter the calculation.

The determination of the PDFs requires a variety of data sets which constrain different linear combinations of the PDF flavors. For example, Neutral Current (NC) charged-lepton Deeply Inelastic Scattering (DIS) (at low $Q^{2}$ ) probes a charge weighted combination $\sim 4 u+d+s+4 c$. In contrast, charged current (CC) neutrino DIS can probe different flavor combinations via $W^{ \pm}$-boson exchange; additionally the neutrino measurements can probe the parity-violating $x F_{3}$ structure function.

## Nuclear Correction Factors

The most precise determination of the strange quark PDF component comes from neutrino-nucleon ( $\nu-\mathrm{N}$ ) di-muon DIS ( $v N \rightarrow \mu^{-} \mu^{+} X$ ) process. This (dominantly) takes place via the Cabibbo favored partonic
process $v s \rightarrow \mu^{-} c$ followed by a semi-leptonic charm decay. As the neutrino cross section is small, this measurement is typically made using heavy nuclear targets ( $\mathrm{Fe}, \mathrm{Pb}$ ), so nuclear corrections must be applied to relate the results to a proton or isoscalar nuclei.

However, recent analyses indicate that the nuclear corrections for the $v$-N and $\ell^{ \pm}-\mathrm{N}$ DIS processes are different [1]; hence, this introduces an uncertainty into the strange quark PDF extraction which was not realized previously. Figure 2 displays the nuclear correction factors obtained for the a) $\ell^{ \pm}-\mathrm{N}$ and b$) ~ v-\mathrm{N}$ processes. Here, we plot the ratio of $F_{2}^{F e}$ to an isoscalar $F_{2}^{N}$ as a function of $x$ for the $Q^{2}$ value indicated.

The contrast between the charged-lepton $\left(\ell^{ \pm} A\right)$ case and the neutrino ( $v A$ ) case in Figure 2 is striking; while the charged-lepton results generally align with the SLAC/NMC [2], KP [3, 4] and HKN [5] determinations, the neutrino results clearly yield different behavior in the intermediate $x$-region. We emphasize that both the charged-lepton and neutrino results are not a model-they come directly from global fits to the data. To emphasize this point, we have superimposed illustrative data points in the figures; these are simply a) the SLAC and BCDMS data $[6,7,8,9,10,11,12]$ or b) the $v A$ DIS data [13] scaled by the appropriate structure function, calculated with the proton PDF of Ref. [2].

The mis-match between the results in charged-lepton and neutrino DIS is particularly interesting given that there has been a long-standing "tension" between the light-target charged-lepton data and the heavy-target neutrino data in the historical fits [14, 15]. This study demonstrates that the tension is not only between charged-lepton light-target data and neutrino heavy-target data, but we now observe this phenomenon


Figure 3: The a) gluon $x g\left(x, Q_{0}\right)$ and b) strange quark $x s\left(x, Q_{0}\right)$ nuclear PDFs as a function of $x$ for a selection of nuclear A values $\{1,2,4,9,12,27,56,108,207\}$ (from top to bottom at $x=0.01$ ). We choose $Q_{0}=1.3 \mathrm{GeV}$.
in comparisons between neutrino and charged-lepton heavy-target data.

## The nCTEQ PDFs

The above example underscores the importance of a comprehensive treatment of the nuclear corrections to achieve the precision demanded by the current precision data. To move toward this goal, the nCTEQ project was developed to extend the global analysis framework of the traditional CTEQ proton PDFs to incorporate a broader set of nuclear data thereby extracting the PDFs of a nuclear target. In essence, a nuclear PDF not only depends on the momentum fraction $x$ and energy scale $Q$, but also on the nuclear " A " value: $f(x, Q, A)$. The structure of the nCTEQ analysis is closely modeled on that of the proton global analysis; in fact, the nuclear parameterizations are designed efficiently to make use of the proton limit $(\mathrm{A}=1)$ as a "boundary condition" to help constrain the fit.

In Figure 3 we display the gluon and strange nuclear PDFs as a function of $x$ for a selection of nuclear A values. We observe that for $x \simeq 0.01$ the nuclear modifications for the strange quark can be $\sim 25 \%$, and for the gluon can be even larger. The details of the nuclear PDF analysis is discussed in Refs. [1, 16, 2] ${ }^{2}$

The nCTEQ web-page contains 19 families of nPDF grid files which may be used to explore the variation due to the different data sets and kinematic cuts. In particular, there is a collections of nPDFs which interpolate between that of Figure 2-a) which uses the charged-lepton-nucleus ( $\ell^{ \pm} A$ ) data and of Figure 2-b) which uses the neutrino-nucleus $(v A)$ data.

[^97]

Figure 4: $\kappa(x)$ vs. $x$ for $Q=1.5 \mathrm{GeV}$ for a selection of PDFs, where we define $\kappa(x)=2 s(x) /(\bar{u}(x)+\bar{d}(x))$

## The Strange Quark PDF

We now compare a selection of $s(x)$ distributions to gain a better understanding of the uncertainties arising from the nuclear correction factors used to analyze the $v \mathrm{~N}$ DIS. One measure of the strange quark content of the proton is to compare $s(x)$ with the average up-quark and down-quark sea PDFs: $(\bar{u}(x)+\bar{d}(x)) / 2$. Thus, we define the ratio $\kappa(x)=2 s(x) /(\bar{u}(x)+\bar{d}(x))$. If we had exact $S U(3)$ flavor symmetry, we would expect $\kappa=1$; the extent to which $\kappa$ is below one measures the suppression of the strange quark as compared to the up and down sea. In Figure 4 we display $\kappa(x)$ for some recent CTEQ PDFs and note that $\kappa(x)$ has a large variation, especially at small $x$ values. This reflects, in part, the fact that the strange quark is poorly constrained for $x \lesssim 0.1$. For the CTEQ6, 6HQ, 6.1, and 6.5 PDF sets, the strange quark was arbitrarily set to $\sim 1 / 2$ the average of the up and down sea-quarks. For the CTEQ6.6 PDF set, the strange quark was allowed additional freedom; this is reflected in Figure 5 which compares the relative uncertainty of the strange quark in the 6.1 and 6.6 PDF sets.


Figure 5: Relative uncertainty of the strange quark PDF as a function of $x$ for $Q=2 \mathrm{GeV}$. The inner band is for the CTEQ6.1 PDF set, and the outer band is for the CTEQ6.6 PDF set. The band is computed as $s_{i}(x) / s_{0}(x)$ where $s_{0}(x)$ is the central PDF for each set; for CTEQ6.1, $i=[1,40]$, and for CTEQ6.6, $i=[1,44]$.


Figure 6: The differential cross section $(d \sigma / d y)$ for $W^{+}$production at the LHC $(\sqrt{s}=14 \mathrm{TeV})$ as a function of rapidity $y$. The partonic contributions are also displayed. At $y=0$, the contributions (from top to bottom) are $\{$ total, $u \bar{d}, c \bar{s}, u \bar{s}, c \bar{d}\}$

## $W / Z$ at the LHC

The above reexamination of the nuclear corrections introduces additional uncertainties into the data sets, which manifests itself in increased uncertainties on the strange quark PDF. To see how these uncertainties might affect other processes, we consider, as an example, $W / Z$ production at the LHC. As we go to higher energies, the heavy quarks will play an increasingly important role because we can probe the PDFs at smaller $x$ and larger $Q$; this means that the heavy quark PDF uncertainties can have an increased influence on LHC observables compared to Tevatron observables.

In Figure 6 we display the LO differential cross section for $W$ production at the LHC as a function of rapidity $y$, as well as the individual partonic contributions. We note that in the central rapidity region the contribution from the heavy quarks can be $30 \%$ or more of the total cross section; this is in sharp contrast to the sit-
uation at the Tevatron where the heavy quark contributions are minimal. Thus, a large uncertainty in the heavy quark PDFs can influence such "benchmark" processes as $\mathrm{W} / \mathrm{Z}$ production at the LHC. Of course, given the high statistics from the LHC (the 2011 proton-proton run exceeded $5 \mathrm{fb}^{-1}$ ), it may be possible to turn the question around and ask to what extent the LHC data may constrain the heavy quark PDFs.

## Zero Mass (ZM) and General Mass (GM) Schemes

We now turn to charm production and the measurement of the charm PDF. HERA extracted precise measurements of $F_{2}^{c}$ and $F_{2}^{b}$, and recently these analyses have been updated ${ }^{3}$ to include the low $Q^{2}$ data to cover the kinematic range of $Q^{2}=[2,1000] \mathrm{GeV}^{2}$ and $x$ down to $10^{-5}[17,18]$.

A global fit of HERA I data $[19,20]$ for $F_{2}^{c}$ was performed using both the General Mass Variable Flavor Scheme (GM-VFS), and also the Zero Mass Variable Flavor Scheme (ZM-VFS). [21] While the GM-VFN result yielded an improved $\chi^{2}$, the ZM-VFN results-when implemented consistently-yielded an acceptable fit to the data. Given the expanded kinematic coverage of the recent HERA data, it would be of interest to repeat this comparison. Presumably the new data sets would allow for increased differentiation between the ZM-VFN and GM-VFN scheme results.

## Choice of Theoretical Schemes

Having illustrated the impact of different theoretical schemes on the data analysis, we take a moment to compare and contrast some of the different schemes that are currently being used for various PDF analysis efforts. While many of the global analyses use a Variable Flavor Number (VFN) scheme to include the heavy quark as a parton, the detailed implementation of this scheme can lead to notable differences. At the 2009 Les Houches workshop, a comparison was performed among a number of the different programs to quantify these differences. All programs used the same PDFs and $\alpha_{S}$ values so that the differences would only reflect the particular scheme. The complete details can be found in Ref. [22], and Figures 7 and 8 display sample comparisons.

Figure 7 compares the S-ACOT scheme which is used for the CTEQ series of global analyses, [23, 24] and the FONLL which is used by the Neural Network PDF (NNPDF) collaboration. [25] In the figure, these two

[^98]

Figure 7: Comparison of $F_{2}^{c}$ for the Fixed-Order-Next-to-LeadingLog (FONLL) with the Simplified-ACOT (S-ACOT) scheme. There are four curves displayed, two for the ordinary $\chi$-rescaling, and two for an alternate $\chi$-rescaling (labeled " v 2 "). The FONLL and S-ACOT results are identical throughout the $x$ range. (Figure from Ref. [22].)


Figure 8: Comparison of $F_{2}^{c}$ for the Fixed-Order-Next-to-LeadingLog (FONLL) and the MSTW08 NLO results. The FONLL results are shown for both the " A " and " B " variations. The FONLL results differ from the MSTW08 results for low $Q$ and $x$; for larger values of $Q$ and $x$ they are more comparable. (Figure from Ref. [22].)
implementations (S-ACOT and FONLL-A) are numerically equivalent.

Figure 8 compares two variations of the FONLL scheme ("A" and "B") with the MSTW08 results which is used in the MSTW series of PDF global analyses. [26, 27] Here these differences reflect the different organization and truncation of the perturbation expansion; it does not indicate that one choice is right or wrong. We expect such differences to be proportional to $\sim \alpha_{S}^{N} \times O\left(m^{2} / Q^{2}\right)$. Thus, as we increase the order of perturbation theory or the energy scale the differences should decrease; we have explicitly verified the difference is reduced as $Q^{2}$ increases, as it should. When we are able to carry these calculations out to higher orders, the scheme differences should be further reduced; this work is in progress.

## Charm Mass Dependence and $\boldsymbol{F}_{\mathbf{2}}^{\boldsymbol{c}}$

The experimental extraction of the "inclusive" $F_{2}^{c}$ requires a differential NLO calculation of DIS charm production to be extrapolated over the unobserved kinematic regions. These analyses generally make use of the HVQDIS program [28] which computes $F_{2}^{c}$ in a Fixed-Flavor-Number (FFN) scheme at NLO. In this calculation, the charm is produced only via a gluon splitting, $g \rightarrow c \bar{c}$, and there is no charm PDF. Thus, the charm mass $\left(m_{c}\right)$ enters only the partonic cross section $\hat{\sigma}\left(m_{c}\right)$ and the final state phase space; there is no PDF charm threshold.

Although we would also like to perform the extraction of $F_{2}^{c}$ using a Variable-Flavor-Number (VFN) scheme, the challenge is that no NLO differential program exists for this process. In lieu of a VFN extraction, another avenue is to study the influence of different theoretical schemes and $m_{c}$ parameters in the analysis of the $F_{2}^{c}$ data. We describe such a study below.

In many analyses, the value of the charm mass is taken as an external fixed parameter. A recent investigation has taken a closer look at the role of the charm mass parameter $m_{c}$ and examined the combined effects of $m_{c}$ and the theoretical scheme used; preliminary results of this study are displayed in Figure 9. For each of the schemes listed in the legend, fits were generated for fixed $m_{c}$ values in the range $[1.2,1.8] \mathrm{GeV}$. Thus, the minimum of the $\chi^{2}$ curve represents the "optimal" choice of the charm mass parameter $m_{c}$ for that specific scheme.

We observe that the various schemes prefer $m_{c}$ values ranging from 1.2 to 1.7 GeV , The largest $m_{c}$ value $(1.68 \mathrm{GeV})$ comes from the Zero Mass VFN Scheme (ZM VFNS) which only uses $m_{c}$ for the PDF charm


Figure 9: Comparison of $\chi^{2}$ for HERAPDF1.0 $+F_{2}^{c \bar{c}}$ fits using different heavy flavor schemes as a function of the charm quark mass parameter $m_{c}^{\text {model }}$. (Figure from Hlprelim-10-143 \& ZEUS-prel-10019)
threshold; it is absent in the phase space for the zeromass case. In contrast, for the S-ACOT- $\chi$ scheme the " $\chi$ " notation ${ }^{4}$ indicates there are effectively two factors of $m_{c}$ in the final phase space, and this yields the smallest value of $m_{c}(1.26 \mathrm{GeV})$.

The ACOT scheme and the Roberts-Thorne (RT) scheme yield $m_{c}$ values in the intermediate region. The ACOT scheme uses the full kinematic mass relations in the partonic relations, and the scaling variable is intermediate ( $m_{c}=1.58 \mathrm{GeV}$ ) between the ZM VFN scheme and the S-ACOT- $\chi$ scheme. The S-ACOT scheme (not shown) is virtually identical to the full ACOT scheme, and also yields a $m_{c}$ value in the intermediate region. Therefore, comparing the S-ACOT$\chi$ and S-ACOT schemes, we find that the $\chi$-rescaling variable is dominantly responsible for the shift of the optimal $m_{c}$ value from $\sim 1.26$ to $\sim 1.58$. This observation suggests that it is the rescaling of the $x$ variable which enters the PDFs that generates the dominant effect. While this study is continuing, it does indicate the sensitivity of the charm mass and scheme choice in these precision analyses.


Figure 10: Measurement of $\gamma+c$ and $\gamma+b$ vs. $P_{T}^{\gamma}$ as measured by D-Zero. (Figure from Ref. [32].)


Figure 11: The integrated momentum fraction (in percent) of the "extrinsic" charm and bottom quarks generated by gluon splitting as a function of the scale $Q$. Reference lines are indicated at $1 \%$ and $2 \%$.

## Extrinsic \& Intrinsic Charm PDFs

The charm quark and bottom quark PDFs can be probed directly at the Tevatron by studying photonheavy quark final states which occur via the sub-process $g Q \rightarrow \gamma Q$ at LO. This process has been measured at the Tevatron for both charm and bottom final states, and we display the results in Figure 10 as a function of $P_{T}^{\gamma}$ for two rapidity configurations. This measurement is particularly interesting as the dominant process involves a heavy quark PDF; this is in contrast to DIS charm or bottom production, for example, where over much of the kinematic range the process is dominated by the gluon-initiated process (e.g., $\gamma g \rightarrow Q \bar{Q}$ ) rather than the heavy quark initiated process $(\gamma Q \rightarrow Q)$.

[^99]

Figure 12: $d \sigma / d p_{T \gamma}(\mathrm{pb} / \mathrm{GeV})$ at the Tevatron for the CTEQ6.6 PDFs, and two intrinsic charm (IC) models. (Figure from Ref. [30].)


Figure 13: Ratio of $d \sigma / d p_{T \gamma}(\mathrm{pb} / \mathrm{GeV})$ at the LHC $(\sqrt{s}=7 T e V)$ for the BPHS IC model to the CTEQ6.6 PDF for a selection of rapidity bins. (Figure from Ref. [30].)

Examining Figure 10 we observe that the bottom quark production measurements compare favorably with the theoretical predictions throughout the $P_{T}^{\gamma}$ range, but the charm results rise above the theory predictions for large $P_{T}^{\gamma}$. Although there may be a number of explanations for the excess charm cross section at large $P_{T}^{\gamma}$, one possibility is the presence of intrinsic charm (IC) in the proton. In the usual DGLAP evolution of the proton PDFs, we begin the evolution at a low energy scale $Q_{0}<m_{c}$ and evolve up to higher scales. The charm and bottom PDFs are defined to be zero for $Q<m_{c, b}$, and above the mass scale the heavy quark PDFs are generated by gluon splitting, $g \rightarrow Q \bar{Q}$; we refer to this as the "extrinsic" contribution to the heavy quark PDFs. In Figure 11 we display the integrated mo-


Figure 14: Measurement of $F_{L}$ using the combined HERA data set from H1 and ZEUS. The data are compared with a selection of theoretical predictions. (Figure H1prelim-10-044 EG ZEUS-prel-10-008).
mentum fractions for the charm and bottom quarks as a function of the scale $Q$; these are zero for $Q<m_{c, b}$, and then begin to grow via the $g \rightarrow Q \bar{Q}$ process.

It has been suggested that there may also be an "intrinsic contribution to the heavy quark PDFs which is present even at low scales $Q<m_{c, b}$. While it is difficult to constrain the detailed functional shape of any intrinsic heavy quark distribution, the total momentum fraction of any intrinsic contribution must be less than approximately $1 \%$ if it is to be compatible with the global analyses.

In Figure 12 we illustrate the effect of including an additional intrinsic charm component in the proton. The BHPS IC model concentrates the momentum fraction at large $x$ values, and the Sea-like IC model distributes the charm more uniformly. ${ }^{5}$ It is intriguing that the IC modification of the proton PDF can increase the theoretical prediction in the large $P_{T}^{\gamma}$ region, but this observation alone is not sufficient to claim the presence of IC; this would require independent verification. In Figure 13 we display the cross section ratio for $\gamma+c$ at the LHC for the BHPS IC model for a selection of rapidity bins. Thus the LHC can validate or refute this possibility with a high-statistics measurement of $\gamma+c$, especially if they can observe this in the forward rapidity region.

## The Longitudinal Structure Function $\boldsymbol{F}_{\boldsymbol{L}}$

Most of the previous discussion has addressed the determination of the quark PDFs. Constraining the gluon PDF is a challenge, and the longitudinal structure function $F_{L}$ is particularly interesting as it involves both the

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Figure 15: Fractional flavor decomposition of $F_{L}^{i} / F_{L}$ vs. $Q$ in GeV for a) $x=10^{-1}$ and b) $x=10^{-5}$. Reading from the bottom, we plot the cumulative contributions for $\{u, d, s, c, b\}$.
heavy quark and the gluon distributions. Using the combined data from H1 and ZEUS, HERA has extracted $F_{L}$ in an extended kinematic regime, and Figure 14 displays the result of the combined data as compared with various theoretical predictions.

The measurement of $F_{L}$ is special for a number of reasons, and we write this schematically as:

$$
\begin{equation*}
F_{L} \simeq \frac{m^{2}}{Q^{2}} q(x)+\alpha_{S}\left\{C_{g} \otimes g(x)+C_{q} \otimes q(x)\right\} \tag{1}
\end{equation*}
$$

Note that the LO term is zero in the limit of massless quarks as the $\left(m^{2} / Q^{2}\right)$ factor in Eq. (1) suppresses the helicity violating contributions; this is a consequence of the Callan-Gross relation. Therefore, for light quarks the dominant contributions come from the NLO gluon term; hence, $F_{L}$ can provide useful information about the gluon PDF.

For the heavy quarks the picture is less obvious. While the NLO heavy quark contributions will clearly be small compared to the dominant gluon terms, the heavy quarks can contribute at LO if they can overcome the $\left(m^{2} / Q^{2}\right)$ suppression. This is why the prediction of $F_{L}$ into the low $Q^{2}$ region as measured in Figure 14 is such a theoretical challenge. This raises a number of questions: What is the flavor composition of $F_{L}$ ? Where are the heavy quark contributions important?

In Figure 15 we display the fractional contributions to the structure functions $F_{L}^{i} / F_{L}$ vs. $Q$. We observe that for large $x$ and low $Q$ the heavy flavor contributions are minimal. For example, in Figure 15-a) at $Q \sim 5 \mathrm{GeV}$ we see the $u$-quark structure function $F_{L}^{u}$ comprises $\sim 80 \%$ of the total, $F_{L}^{d}$ is about $10 \%$, and the $s, c$ and $b$ quarks divide the remaining fraction.

At smaller $x$ values the picture changes and the heavy quarks are more prominent. In Figure 15-b) for $Q \sim$ 2 GeV we see the $u$-quark structure function $F_{L}^{u}$ comprises $\sim 55 \%, F_{L}^{d}$ and $F_{L}^{s}$ are both about $20 \%$, and the $c$ and $b$ quarks make up the small remaining fraction.

However, $F_{L}^{c}$ increases quickly as $Q$ increases and is comparable to $F_{L}^{u}(\sim 40 \%)$ for $Q \sim 20 \mathrm{GeV}$. Additionally, for large $Q \sim 100 \mathrm{GeV}$ we see the contributions of the $u$-quark and $c$-quark are comparable, the $d$-quark and $s$-quark are comparable, and the relative sizes of the $u, c$ to $d, s$ terms are proportional to their couplings: $4 / 9$ to $1 / 9$. Thus, for low $x$ and intermediate to large $Q$ values we see that the quark masses (aside from the top) no longer play a prominent role and we approach the limit of "flavor democracy."

## Concluding Remarks

We reviewed a number of recent developments regarding the extraction and application of heavy quark Parton Distribution Functions (PDFs). The high precision HERA measurements were essential in developing and refining the theoretical treatment of the heavy quarks. Even though the accelerator facility stopped operation four years ago, the analysis of the data continues. The results of these analyses will provide the foundation upon which future PDF analyses will be built, and the advances of the experimental analysis and theoretical tools developed at HERA will continue to influence future hadronic studies including those now beginning at the LHC.

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# Compatibility of global NPDF analyses of neutrino DIS and charged-lepton DIS data 

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The neutrino deep inelastic scattering (DIS) data is very interesting for global analyses of proton and nuclear parton distribution functions (PDFs) since they provide crucial information on the strange quark distribution in the proton and allow for a better flavor decompositon of the PDFs. In order to use neutrino DIS data in a global analysis of proton PDFs nuclear effects need to be understood. We study these effects with the help of nuclear PDFs extracted from global analyses of charged-lepton DIS, Drell-Yan and neutrino DIS data at next-to-leading order in QCD.
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## 1. Introduction

Parton distribution functions are of great importance in contemporary high energy physics. Because they encode fundamental information on the structure of hadrons, PDFs are needed for the computation of any high energy reaction (at HERA, RHIC, Tevatron, LHC, . . . ) involving hadrons in the initial state.

Many groups perform and regularly update global analyses of PDFs for protons [1], , , , 母 ] and nuclei [5, 6, 7]. Although not often emphasized, nuclear effects are present also in the analyses of proton PDFs since a number of experimental data is taken on nuclear targets. Most of the nuclear targets used in the proton analysis are made of light nuclei in which nuclear effects are expected to be small. However, the neutrino DIS data is taken on heavy nuclei such as iron and lead and is sensitive to the strange quark content of the proton. It should be noted that a good knowledge of the strange quark PDF has a significant influence on the $W$ - and $Z$ boson benchmark processes at LHC. Moreover, the neutrino experiments have been used to make precision tests of the Standard Model $(\mathrm{SM})$ in the neutrino sector. A prominent example is the extraction of the weak mixing angle $\sin \theta_{W}$ in a Paschos-Wolfenstein type analysis.

Historically, nuclear corrections based on information from the charged-lepton-nucleus ( $\ell A$ ) DIS data have been applied to the neutrino-nucleus ( $v A$ ) DIS data. Furthermore, the same correction factors have been applied to several different observables in $v A$-DIS ( $F_{2}, F_{3}$, cross section and dimuon production) and at different scales $Q^{2}$. Conversely, it is much more flexible to compute nuclear corrections in the Parton Model (PM) using nuclear PDFs taking different observables and scales into account. For this reason, we perform global analyses of nuclear PDFs at next-to-leading order (NLO) in QCD in a framework closely related to the one used by the CTEQ collaboration in Ref. [9]. We determine several sets of nuclear PDFs from a) $\ell A$ DIS + Drell-Yan (DY) data and b) $v A$ DIS data and c) the combined $\ell A$ DIS $+\mathrm{DY}+v A$ DIS data. We analyze and compare the resulting nuclear correction factors.

## 2. CTEQ Nuclear Parton distribution functions

The global nuclear PDF framework we use to analyze $\ell A$ DIS and DY and $v A$ DIS data was introduced in [ 8$]$. The parameterizations of the parton distributions in bound protons at the input scale of $Q_{0}=1.3 \mathrm{GeV}$

$$
\begin{equation*}
x f_{k}\left(x, Q_{0}\right)=c_{0} x^{c_{1}}(1-x)^{c_{2}} e^{c_{3} x}\left(1+e^{c_{4}} x\right)^{c_{5}} \tag{2.1}
\end{equation*}
$$

where $k=u_{v}, d_{v}, g, \bar{u}+\bar{d}, s, \bar{s}$ and

$$
\begin{equation*}
\bar{d}\left(x, Q_{0}\right) / \bar{u}\left(x, Q_{0}\right)=c_{0} x^{c_{1}}(1-x)^{c_{2}}+\left(1+c_{3} x\right)(1-x)^{c_{4}} \tag{2.2}
\end{equation*}
$$

are a generalization of the parton parameterizations in free protons used in the CTEQ proton analysis [9]. To account for a variety of nuclear targets, we introduce A-dependent fit parameters $c_{k}$

$$
\begin{equation*}
c_{k} \rightarrow c_{k}(A) \equiv c_{k, 0}+c_{k, 1}\left(1-A^{-c_{k, 2}}\right), k=\{1, \ldots, 5\} . \tag{2.3}
\end{equation*}
$$

The free proton PDFs are recovered in this framework in the limit $A \rightarrow 1$. From the input distributions, we can construct the PDFs for a general $(A, Z)$-nucleus

$$
\begin{equation*}
f_{i}^{(A, Z)}(x, Q)=\frac{Z}{A} f_{i}^{p / A}(x, Q)+\frac{(A-Z)}{A} f_{i}^{n / A}(x, Q) \tag{2.4}
\end{equation*}
$$

where the distributions of a bound neutron, $f_{i}^{n / A}(x, Q)$, are related to those of a proton by isospin symmetry.

We performed a global analysis of $\ell A$ DIS + DY data within this framework, determining the $A$-dependence of the parameters $c_{k}(A)$. In this analysis, we applied the same standard kinematic cuts $Q>2 \mathrm{GeV}$ and $W>3.5 \mathrm{GeV}$ as in [9] leaving 708 data points and we obtained a fit with $\chi^{2} /$ dof $=0.946$ with 32 free parameters (for further details see [8]).

To extract the nuclear effects it is useful to define a nuclear correction factor $R$ which is the ratio of the observable $(\mathbf{O})$ using nuclear PDF over free PDF

$$
\begin{equation*}
R[\mathbf{O}]=\frac{\mathbf{O}[\text { nuc. } \mathbf{P D F}]}{\mathbf{O}[\text { free } \mathbf{P D F}]} . \tag{2.5}
\end{equation*}
$$

We compared the nuclear correction factors $R$ for the structure function $\left[F_{2}^{\ell A}\right]$ in $\ell A$ DIS with the structure function $\left[F_{2}^{v A}\right]$ in $v A$ DIS. As first observed in [11], the nuclear correction factor $R\left[F_{2}^{\ell A}\right]$ does not describe the NuTeV $v F e$ data well. This raises the question whether the nuclear corrections in $\ell A$ DIS and $v A$ DIS are different.

For definite conclusions, we set up a global analysis of the combined $\ell A$ DIS $+\mathrm{DY}+v A$ DIS data where we included exclusively the neutrino DIS cross-section data coming from the NuTeV (iron) and Chorus (lead) experiments, respectively. Here we applied the same kinematic cuts as in the first analysis of the charged-lepton data leaving us with 3134 neutrino DIS cross-section data. In a fit to only the neutrino data we obtained a $\chi^{2} /$ dof of 1.33 with 34 free parameters (for further details see [10]).

As expected, the nuclear correction factors using NPDFs extracted from the $v A$ DIS data exhibit clear differences with the corresponding nuclear correction factors using NPDFs extracted from $\ell A$ DIS + DY data which are especially marked at low and intermediate Bjorken $x$.

Analyzing both data sets in a combined global analysis runs into the problem of an imbalance of the number of data points between the two data sets, since the $v A$ DIS data points would be dominant compared to the $\ell A$ DIS and DY data. Therefore, we introduced a weight parameter $w$ to combine the data sets

$$
\begin{equation*}
\chi^{2}=\sum_{l^{ \pm} A \text { data }} \chi_{i}^{2}+\sum_{v A \text { data }} w \chi_{i}^{2} . \tag{2.6}
\end{equation*}
$$

In the case $w=0$, only the $\ell A$ DIS and DY data are included and $w=\infty$ uses only the $v A$ DIS data. Varying the weight $w$, we tried to find a compromise fit which would describe both, $\ell A$ DIS + DY data and $v A$ DIS data, reasonably well. We refer to Table II in [10] for the resulting $\chi^{2}$ of the compromise fits with weights $w=0,1 / 7,1 / 2,1, \infty$ and to Figure 1 in [10] for the corresponding nuclear correction factors. As one can see, with increasing weight $w$ the description of the $\ell A$ DIS data gets worse and the one of the $v A$ DIS data improves.

In order to judge quantitatively on how well the compromise fits describe the data we use the $\chi^{2}$ goodness-of-fit criterion introduced in [12, 2]. We consider a fit to be a good compromise if its $\chi^{2}$ for the $\ell A$ DIS $+\mathrm{DY}+v A$ DIS data is within the $90 \%$ confidence level of the fits to a) only $\ell A$ DIS + DY data and b) only $v A$ DIS data. We define the $90 \%$ percentile $\xi_{90}$ used to define the $90 \%$ confidence level, by

$$
\begin{equation*}
\int_{0}^{\xi_{90}} P\left(\chi^{2}, N\right) d \chi^{2}=0.90 \tag{2.7}
\end{equation*}
$$

where $N$ is the number of degrees of freedom and $P\left(\chi^{2}, N\right)$ is the probability distribution

$$
\begin{equation*}
P\left(\chi^{2}, N\right)=\frac{\left(\chi^{2}\right)^{N / 2-1} e^{-\chi^{2} / 2}}{2^{N / 2} \Gamma(N / 2)} \tag{2.8}
\end{equation*}
$$

We can assign a $90 \%$ confidence level error band to the $\chi^{2}$ of the fits to the $\ell A$ DIS + DY and to the $v A$ DIS data

$$
\begin{equation*}
\chi_{l^{ \pm} A}^{2}=638+45.6, \quad \chi_{v A}^{2}=4192+138 \tag{2.9}
\end{equation*}
$$

Comparing the results of the fits with different weights, listed in Table II in [10], we conclude that there is no good compromise which is compatible with both $90 \%$ confidence level given in Eq. (2.9) (see details in [10]).

## 3. Conclusion

After performing a thorough global NPDF analysis of the combined charged-lepton DIS, DY and neutrino DIS data, we find that nuclear correction factors in $v A$ DIS and $\ell A$ DIS are different and there is no good compromise fit to the combined $\ell A$ DIS, DY and $v A$ DIS data. This has important consequences for global analyses of proton and NPDF, for models explaining the nuclear effects, and precision observables in the neutrino sector. The nCTEQ nuclear PDFs described here as well as the ones obtained in [13] are available at [14].

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# Nuclear corrections in $\nu A$ DIS and their compatibility with global NPDF analyses 

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#### Abstract

We perform a global $\chi^{2}$-analysis of nuclear parton distribution functions using data from charged current neutrino-nucleus ( $\nu A$ ) deep inelastic scattering (DIS), charged-lepton-nucleus ( $\ell^{ \pm} A$ ) DIS, and the Drell-Yan (DY) process. We show that the nuclear corrections in $\nu A$ DIS are not compatible with the predictions derived from $\ell^{ \pm} A$ DIS and DY data. We quantify this result using a hypothesistesting criterion based on the $\chi^{2}$ distribution which we apply to the total $\chi^{2}$ as well as to the $\chi^{2}$ of the individual data sets. We find that it is not possible to accommodate the data from $\nu A$ and $\ell^{ \pm} A$ DIS by an acceptable combined fit. Our result has strong implications for the extraction of both nuclear and proton PDFs using combined neutrino and charged lepton data sets.


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High statistics neutrino deep-inelastic scattering (DIS) experiments have generated significant interest in the literature as they provide crucial information for global fits of parton distribution functions (PDFs). The neutrino DIS data provide the most stringent constraints on the strange quark distribution in the proton, and allow for flavor decomposition of the PDFs which is essential for precise predictions of the benchmark gauge boson production processes at the LHC. Moreover, the neutrino experiments have been used to make precision tests of the Standard Model (SM). A prominent example is the extraction of the weak mixing angle $\theta_{W}$ in a PaschosWolfenstein type analysis [1]. A good knowledge of the neutrino DIS cross sections is also very important for long baseline experiments of the next generation which aim at measuring small parameters of the mixing matrix such as the mixing angle $\theta_{13}$ and eventually the CP violating phase $\delta$.

Due to the weak nature of neutrino interactions the use of heavy nuclear targets is unavoidable, and this complicates the analysis of the precision physics discussed above since model-dependent nuclear corrections must be applied to the data. Our present understanding of the nuclear corrections is mainly based on charged lepton-nucleus ( $\ell A$ ) DIS data. In the early 80's the European Muon Collaboration (EMC) [2] found that the nucleon structure functions $F_{2}$ for iron and deuterium differ. This discovery triggered a vast experimental program to investigate the nuclear modifications of the ratio $R\left[F_{2}^{\ell A}\right]=F_{2}^{\ell A} /\left(A F_{2}^{\ell N}\right)$ for a wide range of nuclear targets with atomic number $A$, see Tab. I. By now, such modifications have been established in a kinematic range from relatively small Bjorken $x\left(x \sim 10^{-2}\right)$ to large $x(x \sim 0.8)$ in the deep inelastic region with squared
momentum transfer $Q^{2}>1 \mathrm{GeV}^{2}$. The behavior of the ratio $R\left[F_{2}^{\ell A}\right]$ can be divided into four regions: (i) $R>1$ for $x \gtrsim 0.8$ (Fermi motion region), (ii) $R<1$ for $0.25 \lesssim x \lesssim 0.8$ (EMC region), (iii) $R>1$ for $0.1 \lesssim x \lesssim 0.25$ (anti-shadowing region), and (iv) $R<1$ for $x \lesssim 0.1$ (shadowing region), with different physics mechanisms explaining the nuclear modifications. The shadowing suppression at small $x$ occurs due to coherent multiple scattering inside the nucleus of a $q \bar{q}$ pair coming from the virtual photon [3] with destructive interference of the amplitudes [4]. The anti-shadowing region is theoretically less well understood but might be explained by the same mechanism with constructive interference of the multiple scattering amplitudes [4] or by the application of momentum, charge, and/or baryon number sum rules. Conversely, the modifications at medium and large $x$ are usually explained by nuclear binding and medium effects and the Fermi motion of the nucleons [5].

Instead of trying to address the origin of the nuclear effects, the data on nuclear structure functions can be analyzed in terms of nuclear PDFs (NPDFs) which are modified as compared to the free nucleon PDFs. Relying on factorization theorems in the same spirit as in the free nucleon case, the advantage of this approach is that the universal NPDFs can be used to make predictions for a large variety of processes in $\ell A, \nu A, p A$, and $A A$ collisions. In addition, the nuclear correction factors required for the interpretation of the neutrino experiments can be calculated in a flexible way, taking into account the precise observable, the nuclear $A$, and the scale $Q^{2}$. The factorization assumption in the nuclear environment is therefore a question of considerable theoretical and practical importance and global analyses of NPDFs based on $\ell A$ DIS and fixed target Drell-Yan (DY) data confirm its

| ID | $\frac{F_{2}^{A}}{F_{2}^{A^{\prime}}}$ | Experiment | \# data | 17 | $\mathrm{Ca} / \mathrm{C}$ | $\begin{aligned} & \text { NMC-95 } \\ & \text { NMC-96 } \end{aligned}$ | $\begin{aligned} & 14 \\ & 15 \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | $\mathrm{He} / \mathrm{D}$ | $\begin{aligned} & \text { SLAC-E139 } \\ & \text { NMC-95,re } \end{aligned}$ | $\begin{gathered} 3 \\ 12 \end{gathered}$ | 18 | $\mathrm{Fe} / \mathrm{C}$ | NMC-95 | 14 |
|  |  |  |  | 19 | Pb/C | NMC-96 | 14 |
| 2 | Li/D | NMC-95 | 11 | 20 | $\mathrm{C} / \mathrm{Li}$ | NMC-95 | 7 |
| 3 | $\mathrm{Be} / \mathrm{D}$ | SLAC-E139 | 3 | 21 | $\mathrm{Ca} / \mathrm{Li}$ | NMC-95 | 7 |
| 4 | C/D | $\begin{aligned} & \text { EMC-88 } \\ & \text { EMC-90 } \\ & \text { SLAC-E139 } \\ & \text { NMC-95,re } \\ & \text { NMC-95 } \\ & \text { FNAL-E665-95 } \end{aligned}$ | 9 <br> 0 <br> 2 <br> 12 <br> 12 <br> 3 | 22 | $\mathrm{He} / \mathrm{D}$ | Hermes | 17 |
|  |  |  |  | 23 | Kr/D | Hermes | 12 |
|  |  |  |  | 24 | $\mathrm{Sn} / \mathrm{C}$ | NMC-96 | 111 |
|  |  |  |  | 25 | N/D | Hermes | 19 |
|  |  |  |  | 32 | D | NMC-97 | 201 |
| 5 | N/D | BCDMS-85 | 9 |  | Total: |  | 616 |
| 6 | Al/D | $\begin{aligned} & \text { SLAC-E049 } \\ & \text { SLAC-E139 } \end{aligned}$ | $\begin{aligned} & 0 \\ & 3 \end{aligned}$ | ID | $\begin{aligned} & \frac{\sigma_{D Y}^{p A}}{\sigma_{D Y}^{p A}} \\ & \hline \end{aligned}$ | Experiment | $\begin{gathered} \# \\ \text { data } \end{gathered}$ |
|  |  |  |  |  |  |  |  |
| 7 | $\mathrm{Ca} / \mathrm{D}$ | EMC-90SLAC-E139NMC-95,reFNAL-E665-95 | $\begin{gathered} 0 \\ 2 \\ 12 \\ 3 \end{gathered}$ | 26 | C/D | FNAL-E772 | 9 |
|  |  |  |  | 27 | $\mathrm{Ca} / \mathrm{D}$ | FNAL-E772 | 9 |
|  |  |  |  | 28 | $\mathrm{Fe} / \mathrm{D}$ | FNAL-E772 | 9 |
|  |  |  |  | 29 | W/D | FNAL-E772 | 9 |
| 8 | $\mathrm{Fe} / \mathrm{D}$ | BCDMS-85BCDMS-87SLAC-E049SLAC-E139SLAC-E140 | 6 <br> 10 <br> 2 <br> 6 <br> 0 | 30 | $\mathrm{Fe} / \mathrm{Be}$ | FNAL-E866 | 28 |
|  |  |  |  | 31 | W/Be | FNAL-E866 | 28 |
|  |  |  |  |  | Total: |  | 92 |
|  |  |  |  |  |  |  |  |
| 9 | $\mathrm{Cu} / \mathrm{D}$ | EMC-88 | 9 | ID | $\frac{d \sigma^{\nu} A}{d x d y}$ | Experiment | $\begin{gathered} \# \\ \text { data } \\ \hline \end{gathered}$ |
|  |  | EMC-93 | 9 | 33 | Pb | CHORUS $\nu$ | 412 |
|  |  | EMC-93 | 9 | 34 | Pb | CHORUS $\bar{\nu}$ | 412 |
| 10 | Ag/D | SLAC-E139 | 2 | 35 | Fe | NuTeV $\nu$ | 1170 |
| 11 | Sn/D | EMC-88 | 8 | 36 | Fe | NuTeV $\bar{\nu}$ | 966 |
| 12 | Xe/D | FNAL-E665-92 | 2 | 37 | Fe | CCFR di- $\mu$ | 44 |
| 13 | $\mathrm{Au} / \mathrm{D}$ | SLAC-E139 | 3 | 38 | Fe | NuTeV di- $\mu$ | 44 |
| 14 | $\mathrm{Pb} / \mathrm{D}$ | FNAL-E665-95 | 3 | 39 | Fe | CCFR di- $\mu$ | 44 |
| 15 | $\mathrm{Be} / \mathrm{C}$ | NMC-96 | 14 | 40 | Fe | NuTeV di- $\mu$ | 42 |
| 16 | Al/C | NMC-96 | 14 |  | Total: |  | 3134 |

Table I. The charged lepton DIS data sets together with DY and with neutrino DIS data sets used in the fit. The table details the specific nuclear targets, and the number of data points with kinematical cuts $\left(Q^{2}>4 G e V^{2}, W>3.5 G e V\right)$. References for the data sets are cited in Refs. [6, 7]
validity in the presently explored kinematic range.
However, in a recent analysis [6] of $\nu F e$ DIS data from the NuTeV collaboration we found that the nuclear correction factors are surprisingly different from the predictions based on the $\ell^{ \pm} F e$ charged-lepton results with important implications for global analyses of proton PDFs. This is not completely unexpected since the structure functions in charged current (CC) neutrino DIS and neutral current (NC) electron/muon DIS are distinct observables with different parton model expressions. From this perspective it is clear that the nuclear correction factors will not be exactly the same even for a universal set of

| $w$ | $l^{ \pm} A$ | $\chi^{2}(/ \mathrm{pt})$ | $\nu A$ | $\chi^{2}(/ \mathrm{pt})$ | total $\chi^{2}(/ \mathrm{pt})$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| 0 | 708 | $638(0.90)$ | - | - | $638(0.90)$ |
| $1 / 7$ | 708 | $645(0.91)$ | 3134 | $4710(1.50)$ | $5355(1.39)$ |
| $1 / 2$ | 708 | $680(0.96)$ | 3134 | $4405(1.40)$ | $5085(1.32)$ |
| 1 | 708 | $736(1.04)$ | 3134 | $4277(1.36)$ | $5014(1.30)$ |
| $\infty$ | - | - | 3134 | $4192(1.33)$ | $4192(1.33)$ |

Table II. Summary table of a family of compromise fits.

NPDFs. Note also that some models in the literature predict differences between reactions in CC and NC DIS [8]. What is, however, unexpected is the degree to which the $R$ factors differ between the structure functions $F_{2}^{\nu F e}$ and $F_{2}^{\ell F e}$. In particular the lack of evidence for shadowing in neutrino scattering down to $x \sim 0.02$ is quite surprising.

The study in Ref. [6] left open the question, whether the neutrino DIS data could be reconciled with the charged-lepton DIS data by a better flavor separation of the NPDFs. In this letter, we address this question in the $A$-dependent framework of Ref. [7] by performing a global $\chi^{2}$-analysis of the combined data from $\nu A$ DIS, $\ell A$ DIS and the DY process listed in Table I.

When combining neutrino and charged-lepton + DY data into a compromise fit, we introduce a weight parameter $w$ into the $\chi^{2}$ via:

$$
\begin{equation*}
\chi^{2}=\sum_{l^{ \pm} A \text { data }} \chi_{i}^{2}+\sum_{\nu A \text { data }} w \chi_{i}^{2} . \tag{1}
\end{equation*}
$$

The $w$ factor allows us to adjust for the different number of points in the separate data sets, and provides a parameter that interpolates between the $\nu A$ and the $\ell^{ \pm} A+\mathrm{DY}$ data. We should stress that the $\chi^{2}$ cited in Table II and also in the text is the standard $\chi^{2}$; Eq. (1) is only used internally in the fitting procedure. We construct a set of compromise fits with weights $w=\left\{0, \frac{1}{7}, \frac{1}{2}, 1, \infty\right\}$ and study the dependence of the result on this weight. The fit to only neutrino data, denoted $w=\infty$ in Table II, is compatible with the results in [6]. Similarly, the fit to only charged-lepton + DY data, denoted $w=0$, agrees well with the analysis in [7].

We first compute the nuclear correction factors $R\left[F_{2}^{\ell F e}\right] \simeq F_{2}^{\ell F e} / F_{2}^{\ell N}$ and $R\left[F_{2}^{\nu F e}\right] \simeq F_{2}^{\nu F e} / F_{2}^{\nu N}[10]$ in the QCD parton model at next-to-leading order employing the NPDF fits in Tab. II for the numerator and free nucleon PDFs for the denominator. The $x$-dependence of $R\left[F_{2}^{\ell F e}\right]$ and $R\left[F_{2}^{\nu F e}\right]$ is shown in Fig. 1 a) and b), respectively, at $Q^{2}=5 \mathrm{GeV}^{2}$. Similar results hold at $Q^{2}=20 \mathrm{GeV}^{2}$ which we do not present here. We observe that the fit to only $\ell A$ DIS + DY data $(w=0)$ well describes the SLAC and BCDMS points in Fig. 1 a). The same is true for the fit to only $\nu A$ DIS data $(w=\infty)$ which is compatible with the results from the NuTeV experiment [9] exemplified in Fig. 1 b). However, comparing the results obtained with the $w=0$ and the


Figure 1. Predictions from the compromise fits for the nuclear correction factors $R\left[F_{2}^{\ell F e}\right] \simeq F_{2}^{\ell F e} / F_{2}^{\ell N}$ (left) and $R\left[F_{2}^{\nu F e}\right] \simeq$ $F_{2}^{\nu F e} / F_{2}^{\nu N}$ (right) as a function of $x$ for $Q^{2}=5 \mathrm{GeV}^{2}$. The data points displayed in figure a) are from BCDMS and SLAC experiments (for references see [7]) and those displayed in figure b) come from the NuTeV experiment [9].
$w=\infty$ fits one can see that they predict considerably different $x$-shapes.

The fits with weights $w=\left\{\frac{1}{7}, \frac{1}{2}, 1\right\}$ interpolate between these two incompatible solutions. As can be seen in Fig. 1 a) and b), with increasing weight the description of the $\ell F e$ data is worsened in favor of a better agreement with the $\nu F e$ points. This trend clearly demonstrates that the $\ell F e$ and the $\nu F e$ data pull in opposite directions. We identify the fits with $w=1 / 2$ or $w=1$ as the best candidates for a possible compromise.

To be able to decisively accept or reject the compromise fits, we apply a statistical goodness-of-fit criterion [11-13] based on the probability distribution for the $\chi^{2}$ given that the fit has $N$ degrees of freedom:

$$
\begin{equation*}
P\left(\chi^{2}, N\right)=\frac{\left(\chi^{2}\right)^{N / 2-1} e^{-\chi^{2} / 2}}{2^{N / 2} \Gamma(N / 2)} \tag{2}
\end{equation*}
$$

This allows us to define the percentiles $\xi_{p}$ via $\int_{0}^{\xi_{p}} P\left(\chi^{2}, N\right) d \chi^{2}=p \%$ where $p=\{50,90,99\}$. Here, $\xi_{50}$ serves as an estimate of the mean of the $\chi^{2}$ distribution and $\xi_{90}$, for example, gives us the value where there is only a $10 \%$ probability that a fit with $\chi^{2}>\xi_{90}$ genuinely describes the given set of data. In a global PDF fit, the best fit $\chi^{2}$ value often deviates from the mean value because the data come from different possibly incompatible experiments having unidentified, unknown errors which are not accounted for in the experimental systematic errors. For this reason we rescale the $\xi_{90}$ and $\xi_{99}$ percentiles relative to the best fit $\chi_{0}^{2}$ [11] to define $C_{90}=\chi_{0}^{2}\left(\xi_{90} / \xi_{50}\right)$ and $C_{99}=\chi_{0}^{2}\left(\xi_{99} / \xi_{50}\right)$. This defines our criterion: a fit with a given $\chi^{2}$ is compatible with the best fit with $\chi_{0}^{2}$ at $90 \%(99 \%)$ confidence if $\chi^{2}<C_{90}$ $\left(\chi^{2}<C_{99}\right)$. We apply it to both the total $\chi^{2}$ and the $\chi^{2}$ of the individual data sets.

For the $\ell A$ DIS + DY data we use the fit with $w=0$ as benchmark with $\chi_{0}^{2}=638$ and $N=677$ degrees of freedom (for 708 data points and 31 free parameters). The upper limits on the $\chi^{2}$ at $90 \%$ and $99 \%$ confidence level (C.L.) are then $C_{90}^{l^{ \pm} A}=684$ and $C_{99}^{l^{ \pm} A}=722$. The benchmark fit for the $\nu A$ DIS data $(w=\infty)$ uses 3134 data points with 33 free parameters resulting in $N=$

3101 and one finds $C_{90}^{\nu A}=4330$ and $C_{99}^{\nu A}=4445$. We see that none of the compromise fits satisfies both limits at the $90 \%$ C.L. which is usually used in global analyses of PDFs to define the uncertainty bands. At the $99 \%$ C.L., there are two fits $(w=1 / 2, w=1)$ which are below the $C_{99}^{\nu A}$ limit. However, only the $w=1 / 2$ fit satisfies the corresponding constraint from the chargedlepton benchmark fit.

We now apply our criterion also to the individual data sets with IDs between 1 and 40 in Table I. For the $\ell A$ DIS + DY data (ID $=[1,31]$ ) we determine the $31 C_{90}\left(C_{99}\right)$ limits by using the individual $\chi_{i}^{2}$ of the $w=0$ fit as $\chi_{0, i}^{2}$. For the $\nu A$ DIS data ( $\mathrm{ID}=[33,40]$ ) we proceed in a similar manner using the individual $\chi_{i}^{2}$ of the $w=\infty$ fit. The results of this detailed analysis are depicted in Fig. 2, where we show the quantity

$$
\begin{equation*}
\frac{\Delta \chi^{2}}{\Delta C_{90}}=\frac{\chi_{i}^{2}-\chi_{0, i}^{2}}{C_{90, i}-\chi_{0, i}^{2}} \quad(i=1, \ldots, 40) \tag{3}
\end{equation*}
$$

where $\chi_{i}^{2}$ represents the $\chi^{2}$-value of the $i$ 'th data set. In cases where $\chi_{i}^{2}>C_{90, i}$ the fit is not compatible with the best fit at the $90 \%$ level and $\Delta \chi^{2} / \Delta C_{90}>1$. The exact $90 \%$ C.L. limit is shown as a constant solid line and the dotted line represents the $99 \%$ confidence limit. The local application of the $\chi^{2}$ hypothesis-testing criterion reveals that even the compromise fit with weight $w=\frac{1}{2}$ which was considered acceptable at the $99 \%$ C.L. when looking at the nuclear correction factors and at the global change in $\chi^{2}$, cannot be accepted as a compromise solution as both the charged-lepton and neutrino DIS data on iron exceed the $99 \%$ limit.
In conclusion, the tension between the $\ell^{ \pm} F e$ and $\nu F e$ data sets leaves us with no possible compromise fit when investigating the results in detail, not even when using the $99 \%$ percentile as the limit as opposed to the more restrictive $90 \%$ limit which is usually used to construct the error PDFs. This detailed analysis confirms the preliminary conclusions of Refs. [6, 7] that there is no possible compromise fit which adequately describes the neutrino DIS data along with the charged-lepton data.

At face value, this conclusion differs from some results in the literature which argue the $\nu A$ and $\ell^{ \pm} A$ data are in



Figure 2. $\Delta \chi^{2} / \Delta C_{90}$ as defined in Eq. (3) for the 40 individual data sets. Results are shown for the $w=\frac{1}{2}$-fit (left) and the fit 'Ucor5' (right) with $w=1$. The solid and dashed lines indicate the $90 \%$ and $99 \%$ confidence limits. The highlighted data sets correspond to DIS $\ell^{ \pm} F e(\mathrm{ID}=8), \nu F e(\mathrm{ID}=35)$, and $\bar{\nu} F e(\mathrm{ID}=36)$.
accord [14]. Here, we believe an essential element in our analysis is the use of the correlated systematic errors of the $\nu A$ data. To highlight this point, we now repeat our analysis, but we combine the statistical and all systematic errors in quadrature (thereby neglecting the information contained in the correlation matrix) for $\nu A$ data for the $w=1$ fit with $Q^{2}>4 G e V$ (as before); we denote this the "Ucor 4 " fit, and we obtain $\chi^{2} / p t$ of 1.14 for $\ell^{ \pm} A$ and 1.00 for $\nu A$. We also use a $Q^{2}>5 \mathrm{GeV}$ fit (denoted "Ucor5") to mimic the cuts of Ref. [14]; here we obtain $\chi^{2} / p t$ of 1.14 for $\ell^{ \pm} A$ and 0.96 for $\nu A$.
If we examine the total $\chi^{2}$ values, we find the $\chi^{2} /$ dof $\sim$ 1 , and might be tempted to conclude we are able to fit both the $\nu A$ and $\ell^{ \pm} A$ data simultaneously. However, if we look at individual data sets and apply our hypothesis testing criteria, the picture is quite different. Fig. 2 b) displays the results for the Ucor5 fit. The higher $Q^{2}$ cut of the Ucor5 fit removes some of the very precise NuTeV data at small- $x$, thus resulting in an improved $\chi^{2}$ compared to Ucor 4 . Nevertheless, many of the $\ell^{ \pm} A$ data sets (ID $=3,4,5,6,8$ ) still lie outside the $99 \%$ CL percentile. Thus, we still conclude that there is no compromise fit for the $\nu A$ and $\ell^{ \pm} A$ data even if we relax the constraints by using uncorrelated errors.

Consequently, the nuclear correction factor for the neutrino DIS data are indeed incompatible with that of the charged lepton DIS and DY data, and this result depends crucially on the use of the precision correlated errors of the neutrino data. This result has important implications for both nuclear and proton PDFs. If we do not know the appropriate nuclear correction to relate different nuclear targets, our ability to extract PDFs is limited. For example, the CTEQ6.6 analysis [15] sidesteps this issues by removing most of the $\nu A$ data from the fit; however, they retain the NuTeV dimuon data since this data is critical to constraining the strange quark PDF. This underscores the importance of the $\nu A$ data for flavor differentiation.

Although the NuTeV data provides the tightest constraints due to their statistics, we note that this issue cannot be tied to a single data set. For example, we find that NuTeV is generally compatible with CCFR and CDHSW[16]. The CHORUS $\nu P b$ and $\bar{\nu} P b$ data have larger uncertainties, so they can be compatible with both
the $\ell^{ \pm} A$ data and the $\mathrm{NuTeV} \nu F e$ data because the $\Delta \chi^{2} / \Delta C_{90}<1$ for all weights. Compared to the theory predictions, NuTeV agrees well in the central $x$ region, but exhibits differences both for low $x$ at low $Q^{2}$, and also for very high $x(x \sim 0.65)$.

We have demonstrated that the $\nu A$ and $\ell^{ \pm} A$ data prefer different nuclear correction factors, and that there is no single "compromise" result that will simultaneously satisfy both data sets. While we have focused on the phenomenological aspects for the present study, this result has strong implications for the extraction of both nuclear and proton PDFs using combined neutrino and chargedlepton data sets. Possibilities include unexpectedly large higher-twist effects, or even non-universal nuclear effects; we leave such questions for a future study.
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# Polarized deeply inelastic scattering (DIS) structure functions for nucleons and nuclei 

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#### Abstract

We extract parton distribution functions (PDFs) and structure functions from recent experimental data of polarized lepton-deeply inelastic scattering (DIS) on nucleons at next-to-leading order (NLO) quantum chromodynamics. We apply the Jacobi polynomial method to the Dokshitzer-Gribov-Lipatov-AltarelliParisi (DGLAP) evolution as this is numerically efficient. Having determined the polarized proton and neutron spin structure, we extend this analysis to describe ${ }^{3} \mathrm{He}$ and ${ }^{3} \mathrm{H}$ polarized structure functions, as well as various sum rules. We compare our results with other analyses from the literature.


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## I. INTRODUCTION

A fundamental challenge of high energy particle physics is to understand the spin structure of protons, neutrons, and nuclei in terms of their parton constituents. The increasing precision of experimental data on inclusive polarized deeply inelastic scattering (DIS) of leptons from nucleons allows us to perform incisive QCD analyses of polarized structure functions to reveal the spin-dependent partonic structure function of the nucleon. Polarized DIS leptonnucleon scattering experiments have been performed at CERN, SLAC, DESY, and JLAB [1-13], and these processes have played a key role in our understanding of QCD and the spin structure of the nucleon [14-18]. There are several comprehensive analyses of the polarized DIS data in the literature [19-44]; this work provides a detailed picture of the spin structure of the nucleons.

The new precision experimental data from the HERMES and COMPASS Collaborations [12,13] of the spin structure function $g_{1}$ provides additional information that we shall use to study the spin structure and quark helicity distributions. We shall choose an approach based on the expansion of orthogonal polynomials; specifically, we will implement Jacobi polynomials as we use experimental data for each bin of $Q^{2}$ separately [43]. Previously [44], we applied the Jacobi polynomials to determine the polarized valon distributions using only the proton experimental data. In this analysis, both the unpolarized and polarized valon distributions were extracted, so more unknown parameters were required as compared to the present analysis. The Jacobi polynomial expansion has also been applied to a variety of QCD analyses [45-66], including the case of polarized parton distribution functions (PDFs) [44,67-73].

[^102]In the present study, we perform a NLO QCD analysis of the polarized deep inelastic data [3-13] in the $\overline{\mathrm{MS}}$ scheme and extract parametrizations of the polarized PDFs and structure functions. In Sec. II, we provide an overview of the Jacobi polynomials approach. In Sec. III we review the parametrization and evolution of the PDFs. In Sec. IV we present the results of our fit to the data, and in Sec. V we compute the associated structure functions and sum rules. Sec. IV contains the conclusions. We also provide an appendix which describes the FORTRAN code which is available.

## II. THE JACOBI POLYNOMIAL METHOD

We perform a NLO fit of the polarized parton distribution functions (PPDFs) using Jacobi polynomials to reconstruct the $x$-dependent quantities from their Mellin moments. The use of Jacobi polynomials has a number of advantages; specifically, it will allow us to factorize the $x$ and $Q^{2}$ dependence in a manner that allows an efficient parametrization and evolution of the structure functions.

For example, if we consider the spin structure function $x g_{1}\left(x, Q^{2}\right)$, we can expand this as

$$
\begin{equation*}
x g_{1}\left(x, Q^{2}\right)=x^{\beta}(1-x)^{\alpha} \sum_{n=0}^{N_{\max }} a_{n}\left(Q^{2}\right) \Theta_{n}^{\alpha, \beta}(x) \tag{1}
\end{equation*}
$$

Here, $\Theta_{n}^{\alpha, \beta}(x)$ are Jacobi polynomials of order $n$, and $N_{\max }$ is the maximum order of our expansion. In this instance, the Jacobi polynomials allow us to factor out the essential part of the $x$ dependence of the structure function into a weight function [45], and the $Q^{2}$ dependence is contained in the Jacobi moments $a_{n}\left(Q^{2}\right)$.

To be more specific, the $x$ dependence of the Jacobi polynomials can be written as

$$
\begin{equation*}
\Theta_{n}^{\alpha, \beta}(x)=\sum_{j=0}^{n} c_{j}^{(n)}(\alpha, \beta) x^{j} \tag{2}
\end{equation*}
$$

where the $c_{j}^{(n)}(\alpha, \beta)$ coefficients are combinations of $\Gamma$ functions involving $\{n, \alpha, \beta\}$. The Jacobi polynomials
satisfy an orthogonality relation with weight function $x^{\beta}(1-x)^{\alpha}$ as follows:

$$
\begin{equation*}
\int_{0}^{1} d x x^{\beta}(1-x)^{\alpha} \Theta_{k}^{\alpha, \beta}(x) \Theta_{l}^{\alpha, \beta}(x)=\delta_{k, l} \tag{3}
\end{equation*}
$$

Thus, given the Jacobi moments $a_{n}\left(Q^{2}\right)$, the polarized structure function $x g_{1}\left(x, Q^{2}\right)$ may be reconstructed from Eq. (1) [44].

We can compute the Jacobi moments $a_{n}\left(Q^{2}\right)$ using the orthogonality relation to invert Eq. (1) to obtain

$$
\begin{align*}
a_{n}\left(Q^{2}\right) & =\int_{0}^{1} d x x g_{1}\left(x, Q^{2}\right) \Theta_{k}^{\alpha, \beta}(x) \\
& =\sum_{j=0}^{n} c_{j}^{(n)}(\alpha, \beta) \mathbf{M}\left[x g_{1}, j+2\right] \tag{4}
\end{align*}
$$

In Eq. (4), we have substituted Eq. (1) for $x g_{1}\left(x, Q^{2}\right)$ and introduced the Mellin transform:

$$
\begin{equation*}
\mathbf{M}\left[x g_{1}, N\right] \equiv \int_{0}^{1} d x x^{N-2} x g_{1}\left(x, Q^{2}\right) \tag{5}
\end{equation*}
$$

We can now relate the polarized structure function $x g_{1}\left(x, Q^{2}\right)$ with its moments [44]

$$
\begin{align*}
x g_{1}\left(x, Q^{2}\right)= & x^{\beta}(1-x)^{\alpha} \sum_{n=0}^{N_{\max }} \Theta_{n}^{\alpha, \beta}(x) \\
& \times \sum_{j=0}^{n} c_{j}^{(n)}(\alpha, \beta) \mathbf{M}\left[x g_{1}, j+2\right] . \tag{6}
\end{align*}
$$

Given Eq. (6) for $x g_{1}\left(x, Q^{2}\right)$, we choose the set $\left\{N_{\text {max }}, \alpha, \beta\right\}$ to achieve optimal convergence of this series throughout the kinematic region constrained by the data. In practice, we find $N_{\max }=9, \alpha=3.0$, and $\beta=0.5$ to be sufficient.

## III. QCD ANALYSIS \& PARAMTRIZATION

## A. Parametrization

We consider a proton comprised of massless partons with helicity distributions $q_{ \pm}\left(x, Q^{2}\right)$ which carry momentum fraction $x$ with a characteristic scale $Q$. The difference $\delta q\left(x, Q^{2}\right)=q_{+}\left(x, Q^{2}\right)-q_{-}\left(x, Q^{2}\right)$ measures how much the parton of flavor $q$ "remembers" of the parent proton polarization. We will parametrize these polarized PDFs at initial scale $Q_{0}^{2}=4 \mathrm{GeV}^{2}$ using the following form:

$$
\begin{equation*}
x \delta q\left(x, Q_{0}^{2}\right)=\mathcal{N}_{q} \eta_{q} x^{a_{q}}(1-x)^{b_{q}}\left(1+c_{q} x\right) \tag{7}
\end{equation*}
$$

where the polarized PDFs are determined by parameters $\left\{\eta_{q}, a_{q}, b_{q}, c_{q}\right\}$, and the generic label $q=\left\{u_{v}, d_{v}, \bar{q}, g\right\}$ denotes the partonic flavors up-valence, down-valence, sea, and gluon, respectively. The normalization constants $\mathcal{N}_{q}$

$$
\begin{equation*}
\frac{1}{\mathcal{N}_{q}}=\left(1+c_{q} \frac{a_{q}}{a_{q}+b_{q}+1}\right) B\left(a_{q}, b_{q}+1\right) \tag{8}
\end{equation*}
$$

are chosen such that $\eta_{i}$ are the first moments of $\delta q_{i}\left(x, Q_{0}^{2}\right)$, $\eta_{i}=\int_{0}^{1} d x \delta q_{i}\left(x, Q_{0}^{2}\right)$, where $B(a, b)$ is the Euler beta function.

The total up and down PDFs are a sum of the valence plus sea distributions: $\delta u=\delta u_{v}+\delta \bar{q}$ and $\delta d=\delta d_{v}+\delta \bar{q}$. We will assume an $S U(3)$ flavor symmetry such that $\delta \bar{q} \equiv$ $\delta \bar{u}=\delta \bar{d}=\delta s=\delta \bar{s}$. While we could allow for an $S U(3)$ symmetry violation term by introducing $\kappa$ such that $\delta s=$ $\delta \bar{s}=\kappa \delta \bar{q}$, as the strange PDF is poorly constrained the results would be insensitive to the specific choice of $\kappa$.

As seen from Eq. (7), each of four polarized parton densities $q=\left\{u_{v}, d_{v}, \bar{q}, g\right\}$ contain four parameters $\left\{\eta_{q}, a_{q}, b_{q}, c_{q}\right\}$ which gives a total of 16 parameters that we must constrain. We now demonstrate that we can eliminate some of these parameters while maintaining sufficient flexibility to obtain a good fit.

## 1. First moments of $\delta u_{v}$ and $\delta d_{v}$

The parameters $\eta_{u_{v}}$ and $\eta_{d_{v}}$ are the first moments of the $\delta u_{v}$ and $\delta d_{v}$ polarized valence quark densities; these quantities can be related to $F$ and $D$ as measured in neutron and hyperon $\beta$ decays according to the relations [74]:

$$
\begin{gather*}
a_{3}=\int_{0}^{1} d x \delta q_{3}=\eta_{u_{v}}-\eta_{d_{v}}=F+D,  \tag{9}\\
a_{8}=\int_{0}^{1} d x \delta q_{8}=\eta_{u_{v}}+\eta_{d_{v}}=3 F-D, \tag{10}
\end{gather*}
$$

where $a_{3}$ and $a_{8}$ are non-singlet combinations of the first moments of the polarized parton densities corresponding to

$$
\begin{gather*}
q_{3}=(\delta u+\delta \bar{u})-(\delta d+\delta \bar{d})  \tag{11}\\
q_{8}=(\delta u+\delta \bar{u})+(\delta d+\delta \bar{d})-2(\delta s+\delta \bar{s}) \tag{12}
\end{gather*}
$$

A reanalysis of $F$ and $D$ with updated $\beta$-decay constants obtained [74] $F=0.464 \pm 0.008$ and $D=0.806 \pm 0.008$. With these values we find

$$
\begin{align*}
& \eta_{u_{v}}=+0.928 \pm 0.014  \tag{13}\\
& \eta_{d_{v}}=-0.342 \pm 0.018 \tag{14}
\end{align*}
$$

We make use of $\eta_{u_{v}}$ and $\eta_{d_{v}}$ to reduce the number of parameters by two.

## 2. Gluon and Sea Quarks

We find the factor $\left(1+c_{q} x\right)$ in Eq. (7) provides flexibility to obtain a good description of the data, particularly for the valence distributions $\left\{u_{v}, d_{v}\right\}$. Thus, we will make use of the $c_{q}$ coefficients for the up-valence and downvalence distributions; in contrast, we are able to set the values for $c_{\bar{q}}$ and $c_{g}$ to zero $\left(c_{\bar{q}}=c_{g}=0\right)$ while maintaining a good fit and eliminating two free parameters. For the parameters $\left\{c_{u_{v}}, c_{d_{v}}\right\}$ we find the fit improves if we use

TABLE I. Final parameter values and their statistical errors in the $\overline{\mathrm{MS}}$ scheme at the input scale $Q_{0}^{2}=4 \mathrm{GeV}^{2}$.

|  | $\eta_{u_{v}}$ | 0.928 ( fixed) |  | $\eta_{\bar{q}}$ | $-0.054 \pm 0.029$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $\delta u_{v}$ | $a_{u_{v}}$ | $0.535 \pm 0.022$ | $\delta \bar{q}$ | $a_{\bar{q}}$ | $0.474 \pm 0.121$ |
|  | $b_{u_{v}}$ | $3.222 \pm 0.085$ |  | $b_{\bar{q}}$ | 9.310 (fixed) |
|  | $c_{u_{v}}$ | 8.180 (fixed) |  | $c_{\bar{q}}$ | 0 |
|  | $\eta_{d_{v}}$ | -0.342 (fixed) |  | $\eta_{g}$ | $0.224 \pm 0.118$ |
| $\delta d_{v}$ | $a_{d_{v}}$ | $0.530 \pm 0.067$ | $\delta g$ | $a_{g}$ | $2.833 \pm 0.528$ |
|  | $b_{d_{v}}$ | $3.878 \pm 0.451$ |  | $b_{g}$ | 5.747 (fixed) |
|  | $c_{d_{v}}$ | 4.789 (fixed) |  | $c_{g}$ | 0 |

$\alpha_{s}\left(Q_{0}^{2}\right)=0.381 \pm 0.017$
$\chi^{2} /$ dof $=273.6 / 370=0.74$
nonzero values, but as these are relatively flat directions in $\chi$-space we shall fix the values as detailed in Table I.

Separately, we find the $b$ parameters control the large- $x$ behavior of the PDFs; thus, the sea quark and gluon distributions have large uncertainties in this region as they are dominated by the valence. To provide some guidance, we observe that for unpolarized parton densities in the large- $x$ region, a ratio of $b_{\bar{q}} / b_{g} \sim 1.6$ provides a good fit. Therefore, we impose this ratio on the polarized $b_{\bar{q}}$ and $b_{g}$ parameters to further reduce the free parameters. Additionally, we are able to extract reasonable constraints on the $a_{\bar{q}}$ and $a_{g}$ parameters; this is a benefit of the Jacobi polynomials.

Having fixed $\left\{\eta_{u_{v}}, \eta_{d_{v}}, c_{\bar{q}}, c_{g}\right\}$ and the ratio $b_{\bar{q}} / b_{g}$ in preliminary minimization, we then set the parameters $\left\{b_{\bar{q}}, b_{g}, c_{u_{v}}, c_{d_{v}}\right\}$ as indicated in Table I; this gives us a total of 9 unknown parameters, in addition to $\alpha_{s}\left(Q_{0}^{2}\right)$.

## B. DGLAP evolution

In the Jacobi polynomial approach the Dokshitzer-Gribov-Lipatov-Altarelli-Parisi (DGLAP) evolution equations are solved in Mellin space. The Mellin transform of the parton densities $q$ are defined analogous to that of Eq. (5):

$$
\begin{align*}
\mathbf{M}\left[\delta q\left(x, Q_{0}^{2}\right), N\right] \equiv & \delta q\left(N, Q_{0}^{2}\right)=\int_{0}^{1} x^{N-1} \delta q\left(x, Q_{0}^{2}\right) d x \\
= & \mathcal{N}_{q} \eta_{q}\left(1+c_{q} \frac{N-1+a_{q}}{N+a_{q}+b_{q}}\right) \\
& \times\left(N-1+a_{q}, b_{q}+1\right), \tag{15}
\end{align*}
$$

where $q=\left\{u_{v}, d_{v}, \bar{q}, g\right\}$, and $B$ is the Euler beta function.
In Mellin space, the twist-2 contributions to the polarized structure function $g_{1}\left(N, Q^{2}\right)$ can be represented in terms of the polarized parton densities and the coefficient functions $\Delta C_{i}^{N}$ by

$$
\begin{align*}
\mathbf{M}\left[g_{1}^{p}, N\right]= & \frac{1}{2} \sum_{q} e_{q}^{2}\left\{( 1 + \frac { \alpha _ { s } } { 2 \pi } \Delta C _ { q } ^ { N } ) \left[\delta q\left(N, Q^{2}\right)\right.\right. \\
& \left.\left.+\delta \bar{q}\left(N, Q^{2}\right)\right]+\frac{\alpha_{s}}{2 \pi} 2 \Delta C_{g}^{N} \delta g\left(N, Q^{2}\right)\right\} . \tag{16}
\end{align*}
$$

Here, the sum runs over quark flavors $\{u, d, s\}$, and $\{\delta q, \delta \bar{q}, \delta g\}$ are the polarized quark, antiquark, and gluon distributions, respectively.

The coefficient functions $\Delta C_{i}^{N}$ are the $N$ th moments of spin-dependent Wilson coefficients, and are given by [16]

$$
\begin{aligned}
\Delta C_{q}^{N}= & \frac{4}{3}\left\{-S_{2}(N)+\left(S_{1}(N)\right)^{2}+\left(\frac{3}{2}-\frac{1}{N(N+1)}\right) S_{1}(N)\right. \\
& \left.+\frac{1}{N^{2}}+\frac{1}{2 N}+\frac{1}{N+1}-\frac{9}{2}\right\} \\
\Delta C_{g}^{N}= & \frac{1}{2}\left[-\frac{N-1}{N(N+1)}\left(S_{1}(N)+1\right)-\frac{1}{N^{2}}+\frac{2}{N(N+1)}\right],
\end{aligned}
$$

with $\quad S_{1}(n)=\sum_{j=1}^{n} \frac{1}{j}=\psi(n+1)+\gamma_{E}, \quad S_{2}(n)=$ $\sum_{j=1}^{n} \frac{1}{j^{2}}=\left(\frac{\pi^{2}}{6}\right)-\psi^{\prime}(n+1), \quad \psi(n)=\Gamma^{\prime}(n) / \Gamma(n), \quad$ and $\psi^{\prime}(n)=d^{2} \ln \Gamma(n) / d n^{2}$.

In summary, we are able to express $x g_{1}^{p}$ in terms of 9 unknown parameters at an input scale of $Q_{0}^{2}=4 \mathrm{GeV}^{2}$. We now examine the fits to the spin structure functions to extract the polarized PDFs from the available data.

## IV. QCD FIT OF $x g_{1}\left(x, Q^{2}\right)$ DATA

Our analysis is performed using the QCD-PEGASUS program [75]. We work at NLO in the QCD evolution using $N_{f}=3$ in the fixed-flavor number scheme with massless partonic flavors $\{u, d, s\}$. We take the renormalization and factorization scales to be equal $\left(\mu_{R}=\mu_{F}\right)$, and we compute the strong coupling $a_{s}\left(Q^{2}\right)$ at NLO using a fourth-order Runge-Kutta integration. Our initial parametrizations (Eq. (7)) are chosen to be invertible in N -space, and this makes our fitting procedure numerically efficient.

For the proton data we use EMC [3], HERMES [5,12], SMC [8], E143 [9], E155 [11] and COMPASS [13], for the neutron data we use E142 [4], HERMES [5,12], and E154 [6,7], and for the deuteron data we use SMC [8], E143 [9], E155 [10], and HERMES [12]. This data is summarized in Table II.

We minimize the global $\chi^{2}[63,66,76]$,

$$
\begin{equation*}
\chi_{\text {global }}^{2}=\sum_{n} w_{n} \chi_{n}^{2}, \tag{17}
\end{equation*}
$$

where the sum $n$ runs over the different experiments, $w_{n}$ is a weight factor for the $n$th experiment, and $\chi_{n}^{2}$ is given by

$$
\begin{equation*}
\chi_{n}^{2}=\left(\frac{1-\mathcal{N}_{n}}{\Delta \mathcal{N}_{n}}\right)^{2}+\sum_{i}\left(\frac{\mathcal{N}_{n} g_{1, i}^{\exp }-g_{1, i}^{\text {theor }}}{\mathcal{N}_{n} \Delta g_{1, i}^{\exp }}\right)^{2} \tag{18}
\end{equation*}
$$

Here, $g_{1, i}^{\exp }, \Delta g_{1, i}^{\exp }$, and $g_{1, i}^{\text {theor }}$ denote the experimental measurement, the experimental uncertainty (statistical and systematic combined in quadrature) and theoretical value for the $i$ th data point, respectively. $\Delta \mathcal{N}_{n}$ is the experimental normalization uncertainty and $\mathcal{N}_{n}$ is an overall normalization factor for the data of experiment $n$. We allow for a relative normalization shift $\mathcal{N}_{n}$ between different

TABLE II. Published data points with the measured $x$ and $Q^{2}$ ranges, the number of data points (with a cut of $Q^{2} \geq 1.0 \mathrm{GeV}^{2}$ ), and the fitted normalization shifts $\mathcal{N}_{i}$.

| Experiment | $x$ range | $Q^{2}$ range $\left[\mathrm{GeV}^{2}\right]$ | \# of data points | $\mathcal{N}_{i}$ |
| :--- | :---: | :---: | :---: | :---: |
| E143 $(p)$ | $0.031-0.749$ | $1.27-9.52$ | 28 | 0.9998 |
| HERMES $(p)$ | $0.028-0.66$ | $1.01-7.36$ | 39 | 1.0006 |
| SMC $(p)$ | $0.005-0.480$ | $1.30-58.0$ | 12 | 0.9999 |
| EMC $(p)$ | $0.015-0.466$ | $3.50-29.5$ | 10 | 1.0094 |
| E155 | $0.015-0.750$ | $1.22-34.72$ | 24 | 1.0226 |
| HERMES06 $(p)$ | $0.026-0.731$ | $1.12-14.29$ | 51 | 0.9992 |
| COMPASS10 $(p)$ | $0.005-0.568$ | $1.10-62.10$ | 15 | 0.9920 |
| Proton |  |  | 179 |  |
| E143 $(d)$ | $0.031-0.749$ | $1.27-9.52$ | 28 | 0.9990 |
| E155 $(d)$ | $0.015-0.750$ | $1.22-34.79$ | 24 | 0.9998 |
| SMC $(d)$ | $0.005-0.479$ | $1.30-54.80$ | 12 | 0.9999 |
| HERMES06 $(d)$ | $0.026-0.731$ | $1.12-14.29$ | 51 | 0.9976 |
| Deuteron |  |  | 115 |  |
| E142 $(n)$ | $0.035-0.466$ | $1.10-5.50$ | 8 | 0.9991 |
| HERMES $(n)$ | $0.033-0.464$ | $1.22-5.25$ | 9 | 0.9999 |
| E154 $(n)$ | $0.017-0.564$ | $1.20-15.00$ | 17 | 0.9996 |
| HERMES06 $(n)$ | $0.026-0.731$ | $1.12-14.29$ | 51 | 1.0000 |
| Neutron |  |  | 85 |  |
| Total |  |  | 379 |  |

data sets within uncertainties $\Delta \mathcal{N}_{n}$ quoted by the experiments.
We minimize the above $\chi^{2}$ value with the 9 unknown parameters plus an undetermined $\alpha_{s}\left(Q_{0}^{2}\right)$. The values of these parameters are summarized in Table I. We find $\chi^{2} /$ d.o.f. $=273.6 / 370$ which yields an acceptable fit to the experimental data.

## V. PDF AND STRUCTURE FUNCTION ANALYSIS

We next present our polarized PDFs and perform comparisons with other recent parametrizations [28,31-34].


FIG. 1 (color online). The polarized parton distribution as function of $x$ and for different values of $Q^{2}$.

## A. Polarized PDFs

Figure 1 displays our polarized PDFs for a selection of $Q^{2}$ values. The up-valence $\left(x \delta u_{v}\right)$ and gluon ( $x \delta g$ ) distributions are positive, while the down-valence ( $x \delta d_{v}$ ) and sea $(x \delta \bar{q})$ distributions are negative. We observe that the evolution shifts all the distributions to smaller values of $x$, and tends to flatten out the peak for increasing $Q^{2}$. Figure 2 displays the extracted NLO polarized PDFs as compared with various parametrizations from the literature [28,38-40].


FIG. 2 (color online). The polarized parton distribution at $Q_{0}^{2}=4 \mathrm{GeV}^{2}$ as a function of $x$. Our fit is the solid curve. Also shown are the results of BB (dashed) [40], DSSV (dasheddotted) [38], GRSV (long dashed-dotted) [28], and AAC (dash-dashed-dotted) [39].

Examining the $x \delta u_{v}$ and $x \delta \bar{q}$ distributions we see that most of the fits are in agreement, with the possible exception of the de Florian-Sassot-Stratmann-Vogelsang (DSSV) [38] curves; for both distributions, the DSSV results approach zero more quickly than the other curves. For the $x \delta d_{v}$ distribution, all of the curves are comparable. The DSSV analysis employs results from semi-inclusive DIS (SI-DIS) data which can impose individual constraints on individual quark flavor distributions in the nucleon [38]. Finally, for the gluon distribution, the DSSV results have a sign change in the region of $x \sim 0.1$ while the other fits are positive. Our result for gluon distribution is located between the DSSV curve and the other fits [28,39,40]. In particular, we find the gluon polarization vanished more quickly for small $x$ values as compared with the other fits; we conjecture that using available asymmetry data in the low $x$ region may contribute to this difference.


FIG. 3 (color online). The polarized structure function $g_{1}^{p}$ as function of $Q^{2}$ in intervals of $x$. The error bars shown are the statistical and systematic uncertainties added in quadrature. Our fit is the solid curve. The values of the shift $\alpha$ are given in parentheses. Also shown are the results of BB (dashed) [31], GRSV (dashed-dotted) [28], LSS (dash-dot-dotted) [34], DNS (dash-dashed-dotted) [33], and AAC (long dashed-dotted) [32].

## B. $g_{1}$ Structure functions

Figure 3 displays results for the polarized structure function $x g_{1}^{p}$. For comparison, we display the results obtained by Blumlein and Bottcher (BB) [31]; Gluck, Reya, Stratmann, and Vogelsang (GRSV) [28]; Leader, Sidorov, Stamenov (LSS) [34]; de Florian, Navarro, Sassot (DNS) [33]; and the Asymmetry Analysis Collaboration (AAC) [32]. There is some spread in the analyses at low values of $x$; however, the data are generally well described within errors. As in the unpolarized case, the presence of scaling violations result a slope that varies with changing $x$ values; this is evident in Fig. 3 where we observe the $Q^{2}$ dependence of the structure function $g_{1}\left(x, Q^{2}\right)$.

Given the polarized proton PDFs, we can use isospin symmetry to obtain the corresponding neutron structure functions. In Fig. 4, we plot the neutron polarized structure function $x g_{1}^{n}$. We also display the NLO QCD curves obtained by Ref. [44] in the polarized valon model (PVM).

We can relate the deuteron structure function to that of the proton and neutron via
$\mathbf{M}\left[g_{1}^{d}, N\right]=\frac{1}{2}\left(1-\frac{3}{2} \omega_{D}\right)\left(\mathbf{M}\left[g_{1}^{p}, N\right]+\mathbf{M}\left[g_{1}^{n}, N\right]\right)$,
where $\omega_{D}=0.05 \pm 0.01$ is the $D$-state wave probability for the deuteron [77]. In Fig. 5 we present our results for the structure functions $x g_{1}^{p}\left(x, Q^{2}\right), x g_{1}^{n}\left(x, Q^{2}\right)$, and $x g_{1}^{d}\left(x, Q^{2}\right)$, and this compares favorably with the results of the BB [31], GRSV [28], LSS [34], DNS [33], and AAC [32] analyses.


FIG. 4 (color online). The polarized structure function $x g_{1}^{n}$ as function of $x$ and for a fixed value of $Q^{2}=5 \mathrm{GeV}^{2}$. The present fit is the solid curve. Also shown are the results of AK [44] (dashed) according to polarized valon model (PVM).


FIG. 5 (color online). The polarized structure function $x g_{1}^{p}, x g_{1}^{n}$ and $x g_{1}^{d}$ as a function of $x$ for selected values of $Q^{2}$. The data are well described by the fit (solid curve). Also shown are the QCD NLO curves obtained by BB (dashed) [31], GRSV (dotted) [28], LSS (dash-dotted) [34], AAC (dash-dot-dotted) [32], and DNS (dash-dash-dotted) [33].


FIG. 6 (color online). The non-singlet polarized structure function $x g_{1}^{N S}$ as function of $x$.

The non-singlet spin structure function $x g_{1}^{N S}\left(x, Q^{2}\right)$ is defined as [12]

$$
\begin{align*}
x g_{1}^{N S}\left(x, Q^{2}\right) & \equiv x g_{1}^{p}\left(x, Q^{2}\right)-x g_{1}^{n}\left(x, Q^{2}\right) \\
& =2\left[x g_{1}^{p}\left(x, Q^{2}\right)-\frac{x g_{1}^{d}\left(x, Q^{2}\right)}{1-\frac{3}{2} \omega_{D}}\right] \tag{20}
\end{align*}
$$

This is displayed in Fig. 6, and we compare with the HERMES data [12] for various $Q^{2}$ bins. In the second line of Eq. (20) we have related the structure function of the deuteron using isospin symmetry and the relation of Eq. (19).

## C. $g_{2}$ Structure function

We can now extract the structure function $x g_{2}$ via the Wandzura-Wilczek relation [78,79]:

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FIG. 7 (color online). The polarized structure function $x g_{2}$ as function of $x$ for $Q^{2}=5 \mathrm{GeV}^{2}$.

$$
\begin{equation*}
g_{2}\left(x, Q^{2}\right)=-g_{1}^{p}\left(x, Q^{2}\right)+\int_{x}^{1} \frac{d y}{y} g_{1}^{p}\left(y, Q^{2}\right) . \tag{21}
\end{equation*}
$$

This relation remains valid in the presence of target mass corrections. In Fig. 7 we show our result for $x g_{2}$ and we compare it with the experimental data from E143 [9] and SMC [8].

## D. First moment of $\boldsymbol{g}_{\boldsymbol{1}}$ structure functions

We next use the polarized PDFs to compute the first moments, and compare with other recent analyses. We can obtain the first moment of $g_{1}^{p}$ by

$$
\begin{equation*}
\Gamma_{1}^{p}\left(Q^{2}\right) \equiv \int_{0}^{1} d x g_{1}^{p}\left(x, Q^{2}\right) \tag{22}
\end{equation*}
$$

The results of our fit are presented in Table III for selected values of $Q^{2}$, and these are compared with results from the literature in Table IV.

In the framework of QCD the spin of the proton can be expressed in terms of the first moment of the total quark

TABLE III. The first moments of polarized parton distributions, $\Delta u_{v}, \Delta d_{v}, \Delta \bar{q}, \Delta g$ and polarized structure functions $\Gamma_{1}^{p}$, $\Gamma_{1}^{n}, \Gamma_{1}^{d}$ in NLO in the $\overline{\mathrm{MS}}$ scheme for some different values of $Q^{2}$.

| $Q^{2}$ | $2 \mathrm{GeV}^{2}$ | $3 \mathrm{GeV}^{2}$ | $5 \mathrm{GeV}^{2}$ | $10 \mathrm{GeV}^{2}$ |
| :--- | ---: | ---: | ---: | ---: |
| $\Delta u_{v}$ | 0.928864 | 0.928310 | 0.927794 | 0.927288 |
| $\Delta d_{v}$ | -0.342318 | -0.342114 | -0.341924 | -0.341738 |
| $\Delta \bar{q}$ | -0.053400 | -0.053893 | -0.054379 | -0.054789 |
| $\Delta g$ | 0.143610 | 0.191313 | 0.248845 | 0.323886 |
| $\Gamma_{1}^{p}$ | 0.128291 | 0.131199 | 0.133822 | 0.136303 |
| $\Gamma_{1}^{n}$ | -0.050972 | -0.052416 | -0.053735 | -0.055000 |
| $\Gamma_{1}^{d}$ | 0.035296 | 0.035965 | 0.036559 | 0.037115 |

TABLE IV. Comparison of the first moments of the polarized parton densities in NLO in the $\overline{\mathrm{MS}}$ scheme at $Q^{2}=4 \mathrm{GeV}^{2}$ for different sets of recent parton parametrizations. The second column ("Model") contains the first moments which are obtained from our new parametrization based on the Jacobi polynomials expansion method. The BB [40], GRSV [28], and AAC [32] results are also shown.

|  | Model | BB [40] | GRSV [28] | AAC [32] |
| :--- | ---: | ---: | ---: | ---: |
| $\Delta u_{v}$ | 0.928 | 0.928 | 0.9206 | 0.9278 |
| $\Delta d_{v}$ | -0.342 | -0.342 | -0.3409 | -0.3416 |
| $\Delta u$ | 0.874 | 0.866 | 0.8593 | 0.8399 |
| $\Delta d$ | -0.396 | -0.404 | -0.4043 | -0.4295 |
| $\Delta \bar{q}$ | -0.054 | -0.062 | -0.0625 | -0.0879 |
| $\Delta g$ | 0.224 | 0.462 | 0.6828 | 0.8076 |

and gluon helicity distributions and their orbital angular momentum, i.e.,

$$
\begin{equation*}
\frac{1}{2}=\frac{1}{2} \Delta \Sigma^{p}+\Delta g^{p}+L_{z}^{p} \tag{23}
\end{equation*}
$$

where $L_{z}^{p}$ is the total orbital angular momentum of all quarks and gluons. The contribution of $\frac{1}{2} \Delta \Sigma+\Delta g$ for typical value of $Q^{2}=4 \mathrm{GeV}^{2}$ is around 0.355 in our analysis. We can also compare this value in NLO with other recent analysis. The reported value from the BB model [40] is 0.569 , the AAC model [32] is 0.837 , and the GRSV model [28] is 0.785 , while the DSSV model [38] is approximately 0.1 . Since the values of $\frac{1}{2} \Delta \Sigma$ are comparable, we observe that the difference between the above reported values must come from different gluon distributions.

## E. Strong coupling constant

In this QCD analysis we extract $\alpha_{s}\left(Q_{0}^{2}\right)$ at NLO and obtain

$$
\begin{equation*}
\alpha_{s}\left(Q_{0}^{2}\right)=0.381 \pm 0.017 \tag{24}
\end{equation*}
$$

Rescaling this to the $Z$ boson mass scale we find

$$
\begin{equation*}
\alpha_{s}\left(M_{Z}^{2}\right)=0.1149 \pm 0.0015 \tag{25}
\end{equation*}
$$

The error given in the above equation does not include the relative systematics of the different classes of measurements. In Table V we provide a comparison of this value with other determinations from the literature computed at NLO and higher orders, including the current world average of $\alpha_{s}\left(M_{Z}^{2}\right)=0.1184 \pm 0.0007$.

## F. Nuclear polarized structure functions

Using the polarized PDF fit results, we examine the nucleon corrections factors for ${ }^{3} \mathrm{He}$ and ${ }^{3} \mathrm{H}$. The polarized structure functions $g_{1}^{3 \mathrm{He}}$ and $g_{1}^{3} \mathrm{H}$ can be composed from the polarized proton structure $g_{1}^{p}$ and the polarized neutron structure $g_{1}^{n}$ as follows:

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TABLE V. Comparison of $\alpha_{s}\left(M_{Z}\right)$ values from the literature.

| $\alpha_{s}\left(M_{Z}^{2}\right)$ | Order | Reference | Notes |
| :--- | :---: | :---: | :---: |
| $0.1149 \pm 0.0015$ | NLO | $\ldots$ | This analysis |
| $0.1132_{-0.0095}^{+0.0056}$ | NLO | $[40]$ | $\ldots$ |
| $0.1134_{-0.0021}^{+0.0019}$ | NNLO | $[80]$ | $\ldots$ |
| $0.1141 \pm 0.0036$ | NLO | $[44]$ | $\ldots$ |
| $0.1131 \pm 0.0019$ | NNLO | $[63]$ | $\ldots$ |
| $0.1139 \pm 0.0020$ | NNNLO | $[66]$ | $\ldots$ |
| $0.1141_{-0.00022}^{+0.0020}$ | NNNLO | $[80]$ | $\ldots$ |
| $0.1135 \pm 0.0014$ | NNLO | $[81]$ | FFS |
| $0.1129 \pm 0.0014$ | NNLO | $[81]$ | BSMN |
| $0.1124 \pm 0.0020$ | NNLO | $[82]$ | dynamic approach |
| $0.1158 \pm 0.0035$ | NNLO | $[82]$ | standard approach |
| $0.1171 \pm 0.0014$ | NNLO | $[83]$ | $\ldots$ |
| $0.1147 \pm 0.0012$ | NNLO | $[84]$ | $\ldots$ |
| $0.1145 \pm 0.0042$ | NNLO | $[85]$ | (Preliminary) |
| $0.1184 \pm 0.0007$ | $\ldots$ | $[86]$ | World Average |

$$
\begin{align*}
g_{1}^{3} \mathrm{He}\left(x, Q^{2}\right)= & \int_{x}^{3} \frac{d y}{y} \Delta f_{{ }_{3} \mathrm{He}}^{n}(y) g_{1}^{n}\left(\frac{x}{y}, Q^{2}\right) \\
& +2 \int_{x}^{3} \frac{d y}{y} \Delta f_{3_{\mathrm{He}}}^{p}(y) g_{1}^{p}\left(\frac{x}{y}, Q^{2}\right) \\
& -0.014\left[g_{1}^{p}\left(x, Q^{2}\right)-4 g_{1}^{n}\left(x, Q^{2}\right)\right],  \tag{26}\\
g_{1}^{{ }^{3} \mathrm{H}}\left(x, Q^{2}\right)= & 2 \int_{x}^{3} \frac{d y}{y} \Delta f_{3_{\mathrm{H}}}^{n}(y) g_{1}^{n}\left(\frac{x}{y}, Q^{2}\right) \\
& +\int_{x}^{3} \frac{d y}{y} \Delta f_{3 \mathrm{H}}^{p}(y) g_{1}^{p}\left(\frac{x}{y}, Q^{2}\right) \\
& +0.014\left[g_{1}^{p}\left(x, Q^{2}\right)-4 g_{1}^{n}\left(x, Q^{2}\right)\right] . \tag{27}
\end{align*}
$$

Here, $\Delta f_{3_{\mathrm{He}}}^{N}(y)$ and $\Delta f_{3_{\mathrm{H}}}^{N}(y)$ are the spin-dependent nucleon light-cone momentum distributions [87,88]. These functions parametrize the Fermi motion and the nucleon binding, and are readily calculated using the ground-state wave functions of ${ }^{3} \mathrm{He}$ and ${ }^{3} \mathrm{H}$. Note that the last term in above equations is important only in the large- $x$ region.

If we utilize isospin symmetry, we can equate $\Delta f_{{ }_{3} \mathrm{He}}^{p}(y)$ to $\Delta f_{{ }_{3} \mathrm{H}}^{n}(y)$, and also $\Delta f_{{ }_{3} \mathrm{He}}^{n}(y)$ to $\Delta f_{{ }_{3} \mathrm{H}}^{p}(y)$; thus, we are left with only two independent functions $\Delta f_{3 \mathrm{He}}^{p}(y)$ and $\Delta f_{{ }_{3} \mathrm{He}}^{n}(y)$. Using the results of Refs. [88-90], we express these distributions as

$$
\begin{gather*}
\Delta f_{{ }_{\mathrm{He}}}^{n}(y)=\frac{a^{n} e^{-\left(0.5\left(1-d^{n}\right)\left(-b^{n}+y\right)^{2} /\left(c^{n}\right)^{2}\right)}}{1+\frac{d^{n}\left(-b^{n}+y\right)^{2}}{\left(c^{n}\right)^{2}}},  \tag{28}\\
\Delta f_{{ }_{\mathrm{He}}}^{p}(y)=\frac{\sum_{i=0}^{4} a_{i}^{p} U_{i}(y)}{\sum_{i=0}^{4} b_{i}^{p} U_{i}(y)}, \tag{29}
\end{gather*}
$$

where $U_{n}(y)$ is a Chebyshev polynomial of the second type. The numerical coefficients of these equations are

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TABLE VI. Numerical coefficients for Eqs. (28) and (29), of $\Delta f_{{ }_{3} \mathrm{He}}^{n}(y)$ and $\Delta f_{{ }_{3} \mathrm{He}}^{p}(y)$ obtained from Refs. [88-90].

| $n$ | $p$ | $p$ |
| :--- | :--- | :--- |
| $a^{n}=5.650556817$ | $a_{0}^{p}=0.0148376$ | $b_{0}^{p}=4.15388$ |
| $b^{n}=0.986818274$ | $a_{1}^{p}=-0.0189575$ | $b_{1}^{p}=-4.75525$ |
| $c^{n}=0.064446823$ | $a_{2}^{p}=0.0121792$ | $b_{2}^{p}=2.68417$ |
| $d^{n}=0.807650292$ | $a_{3}^{p}=-0.0040397$ | $b_{3}^{p}=-0.800306$ |
|  | $a_{4}^{p}=0.000540845$ | $b_{4}^{p}=0.101095$ |

presented in Table VI. We can then use Eqs. (26) and (27) to obtain the polarized nucleon structure functions $g_{1}^{3} \mathrm{He}\left(x, Q^{2}\right)$ and $g_{1}{ }^{3} \mathrm{H}\left(x, Q^{2}\right)$.
To determine the $g_{1}^{3} \mathrm{He}$ and $g_{1}^{3} \mathrm{H}$ polarized structure functions we need the polarized light-cone distribution functions for proton and neutron in ${ }^{3} \mathrm{He}$, i.e., $\Delta f_{3_{\mathrm{He}}}^{p}$ and $\Delta f_{3_{\mathrm{He}}}^{n}$. In Figs. 8 and 9 we present our results using the parametrization of Eqs. (28) and (29), which is based on the numerical results of Ref. [90].


FIG. 8 (color online). The polarized light-cone distribution function for the proton in the ${ }^{3} \mathrm{He}$, based on the results of Ref. [88-90].


FIG. 9 (color online). The polarized light-cone distribution function for the neutron in the ${ }^{3} \mathrm{He}$, based on the results of Ref. [88-90].


FIG. 10 (color online). Analytical result for the polarized ${ }^{3} \mathrm{He}$ structure function v.s. $x$ for fixed $Q^{2}=2.5 \mathrm{GeV}^{2}$. The current fit is the solid curve. Also shown are the QCD NLO curves obtained by AK (dashed) [44] according to polarized valon model (PVM) and BB (dashed-dotted) [31].

In Figs. 10 and 11 we show our results for the $g_{1}{ }^{3} \mathrm{He}$ and $g_{1}^{3} \mathrm{H}$ polarized structure function, and compare with BB [31], and the PVM [44]. For the $g_{1}^{3} \mathrm{He}$ polarized structure function we see that our result coincides with the BB fit for $x$ values down to $\sim 10^{-2}$, and then falls off more quickly at very small $x$ values. The polarized valon model (PVM), while still a reasonable fit to the data, lies below both of the other fits. For the $g_{1}{ }^{3} \mathrm{H}$ polarized structure function, our fit


FIG. 11 (color online). Analytical result for the polarized ${ }^{3} \mathrm{H}$ structure function v.s. $x$ for fixed $Q^{2}=2.5 \mathrm{GeV}^{2}$. The current fit is the solid curve. Also shown are the QCD NLO curves obtained by AK (dashed) [44] according to polarized valon model (PVM) and BB (dashed-dotted) [31] for comparison.
coincides with the BB fit at both large and small $x$ values, but dips below it (closer to the PVM) for intermediate $x$ values. The differences between these curves come from the various data sets used, the constraints imposed, and the form of the parametrization. For example, in the AK fit [44], only 257 experimental data points were used as the neutron data were not included; in contrast, the present analysis uses 379 points which does include the neutron data. Furthermore, the AK fit used 15 free parameters while there are only 9 free parameters in the present analysis. These differences are reflected in the extractions of PPDFs, and a comparison of these different analyses may be indicative of the stability of the determined QCD parameters.

## G. Bjorken sum rule

We can also study the Bjorken sum rule [91] which relates the difference of the first moments of the proton and neutron spin structure functions to the axial vector coupling constant of the neutron $\beta$-decay,
$\int_{0}^{1}\left[g_{1}^{p}\left(x, Q^{2}\right)-g_{1}^{n}\left(x, Q^{2}\right)\right] d x=\frac{1}{6} g_{A}\left[1+O\left(\frac{\alpha_{s}}{\pi}\right)\right]$,
where $g_{A}=1.2670 \pm 0.0035$ [74], and the QCD radiative corrections are denoted as $O\left(\frac{\alpha_{s}}{\pi}\right)$. This sum rule can be generalized for the ${ }^{3} \mathrm{He}-{ }^{3} \mathrm{H}$ system as follows:

$$
\begin{equation*}
\int_{0}^{3}\left[g_{1}^{{ }^{3} \mathrm{H}}\left(x, Q^{2}\right)-g_{1}^{{ }^{3} \mathrm{He}}\left(x, Q^{2}\right)\right] d x=\frac{1}{6} \tilde{g}_{A}\left[1+O\left(\frac{\alpha_{s}}{\pi}\right)\right], \tag{31}
\end{equation*}
$$

where $\tilde{g}_{A}$ is the axial vector coupling constant of the Triton $\beta$ decay, with $\tilde{g}_{A}=1.211 \pm 0.002$ [92]. Taking the ratio of the Eqs. (30) and (31), we find

$$
\begin{equation*}
\frac{\int_{0}^{3}\left[g_{1}^{3} \mathrm{H}\left(x, Q^{2}\right)-g_{1}^{{ }^{3} \mathrm{He}}\left(x, Q^{2}\right)\right] d x}{\int_{0}^{1}\left[g_{1}^{p}\left(x, Q^{2}\right)-g_{1}^{n}\left(x, Q^{2}\right)\right] d x}=\frac{\tilde{g}_{A}}{g_{A}} . \tag{32}
\end{equation*}
$$

Given $g_{A}$ and $\tilde{g}_{A}$, we compute the above ratio to be 0.956 [88]. Note that the QCD radiative corrections are expected to cancel exactly in above equation. Using the Bjorken sum rules of Eqs. (30) and (31), we obtain the value 0.924 for the ratio of Eq. (32).

## VI. CONCLUSIONS

We have presented a fit to the polarized lepton-DIS data on nuclei at NLO QCD using the Jacobi polynomial method. Having extracted the polarized PDFs, we compute various nuclear structure functions $\left(g_{1}, g_{2}\right)$ and Bjorken sum rule. In general, we find good agreement with the experimental data, and our results are in accord with other determinations from the literature; collectively, this demonstrates progress of the field toward a detailed description of the spin structure of the nucleon.

Having demonstrated the compatibility of the Jacobi polynomial method with other approaches in the literature,
this study can serve as a foundation for addressing issues of polarized scattering processes from a complementary perspective. In particular, the Jacobi polynomial method offers the opportunity to examine efficiencies of different methods, and this work is in progress.

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## APPENDIX: FORTRAN CODE

A FORTRAN package containing our $g_{1}\left(x, Q^{2}\right)$ polarized structure functions for $\left\{p, n, d, N S,{ }^{3} \mathrm{He},{ }^{3} \mathrm{H}\right\} \quad$ and $x g_{2}^{p}\left(x, Q^{2}\right)$, as well as the polarized parton densities $\left\{u_{v}, d_{v}, g, \bar{q}\right\} . x \delta u_{v}\left(x, Q^{2}\right), x \delta d_{v}\left(x, Q^{2}\right), x \delta g\left(x, Q^{2}\right)$, and $x \delta \bar{q}\left(x, Q^{2}\right)$ at NLO in the $\overline{\mathrm{MS}}$ scheme, can be found at http://particles.ipm.ir/links/QCD.htm or obtained via email from the authors. These functions are interpolated using cubic splines in $Q^{2}$ and a linear interpolation in $\log \left(Q^{2}\right)$. The package includes an example program to illustrate the use of the routines.
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# Nonsinglet spin-dependent structure functions 

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#### Abstract

We investigate the nonsinglet spin-dependent structure function for polarized deep inelastic scattering (DIS) of leptons on nucleons in the next-to-leading-order (NLO) approximation. We perform a fit to extract the polarized parton distribution functions (PPDFs) and the nonsinglet spin structure function using the most recent proton and neutron DIS data. We demonstrate that our results yield good agreement with available observables.


Keywords: Nonsinglet polarized structure function; DGLAP equation.

## 1. Introduction

The investigation of the short-distance structure of the nucleon spin is a rich and developing field. Nucleons, by virtue of being composite particles, obtain their spin from a combination of the spin and orbital angular momentum of the underlying quarks and gluons. When the European Muon Collaboration (EMC) [1] uncovered the proton spin crisis more than 20 years ago, this stimulated worldwide interest on both the experimental and theoretical side to understand the spin structure of the nucleon. The remarkable growth of experimental measurements of exclusive polarized DIS of leptons in recent years [1-11] allows to perform incisive QCD analyses of the polarized structure functions and reveal the spin-dependent partonic structure of nucleons.

In the present paper we perform a fit of the polarized proton, neutron and deuteron experimental data to extract a new parameterization of the polarized quark and gluon distributions. In this fit, we determine the polarized parton densities together with QCD coupling constant. Finally, we compare our polarized nonsinglet structure functions with available experimental data.
The organization of this paper is as follows. In Section 2 we outline the theoretical background of the

[^103]QCD analysis. The construction of the nonsinglet spindependent structure function is described in Section 3, and Section 4 contains our conclusions.

## 2. Theoretical background of the QCD analysis

The QCD parton model is a versatile tool for the investigation of unpolarized scattering processes [12]. In light of these successes, the parton model has been extended to scattering of polarized particles as well. We consider a proton comprised of massless partons with positive and negative helicity distributions $q_{ \pm}\left(x, Q^{2}\right)$ which carry fractional momentum fraction $x$ with a characteristic scale $Q$. The difference

$$
\begin{equation*}
\delta q\left(x, Q^{2}\right)=q_{+}\left(x, Q^{2}\right)-q_{-}\left(x, Q^{2}\right), \tag{1}
\end{equation*}
$$

measures how much the parton of flavor $q$ "remembers" of the parent proton polarization; there is a corresponding definition for the antiquarks and gluons as well.

At NLO, the spin-dependent structure functions $g_{1}^{p}$ can be written as a linear combination of $\delta q, \delta \bar{q}$, and $\delta g$ :

$$
\begin{align*}
& g_{1}^{p}\left(x, Q^{2}\right)=\frac{1}{2} \sum_{q} e_{q}^{2}\left\{\delta q\left(x, Q^{2}\right)+\delta \bar{q}\left(x, Q^{2}\right)\right. \\
& \left.+\frac{\alpha_{s}\left(Q^{2}\right)}{2 \pi}\left[\delta C_{q} \otimes(\delta q+\delta \bar{q})+2 \delta C_{g} \otimes \delta g\right]\right\}, \tag{2}
\end{align*}
$$

where $\delta C_{q}, \delta C_{g}$ are the spin-dependent quark and gluon Wilson coefficients, and $e_{q}$ are the electric charges of the
light quark-flavors $q=u, d, s$. We choose to work in the $\overline{M S}$ factorization scheme. The functions $g_{1}^{p}$ and $g_{1}^{n}$ differ only in their nonsinglet components that are related though isospin symmetry, which effectively exchanges the $u$ and $d$ quarks.

We now summarize the key features of our QCD analysis. The polarized parton densities are parametrized at a starting scale $Q_{0}$ and evolved to higher factorization scales using a numerical solution of the polarized NLO DGLAP evolution equations. Our calculation is performed with the Fortran package QCD-PEGASUS[13] which provides accurate solutions of the evolution equations for polarized and unpolarized parton distributions of hadrons in perturbative QCD. We choose a starting scale of $Q_{0}=4 \mathrm{GeV}^{2}$, and take the QCD coupling as free parameter which is fit to the data.

The QCD DGLAP equations are solved in Mellin space where the Mellin transform are defined as:

$$
\begin{align*}
\mathbf{M}\left[\delta f_{i}\left(x, Q^{2}\right)\right](N) & =\delta f_{i}\left(N, Q^{2}\right) \\
& =\int_{0}^{1} x^{N-1} \delta f_{i}\left(x, Q^{2}\right) d x \tag{3}
\end{align*}
$$

and

$$
\begin{align*}
\mathbf{M}\left[x g_{1}\left(x, Q^{2}\right)\right](N) & =g_{1}^{p}\left(N, Q^{2}\right) \\
& =\int_{0}^{1} x^{N-2} g_{1}^{p}\left(x, Q^{2}\right) d x \tag{4}
\end{align*}
$$

where $f_{i}=q_{v}, d_{v}, \bar{q}, g$.
Therefore, the leading (twist-2) contributions to the structure function $g_{1}\left(N, Q^{2}\right)$ can be represented in Mellin-N space by [12]

$$
\begin{align*}
& g_{1}^{p}\left(N, Q^{2}\right)=\frac{1}{2} \sum_{q} e_{q}^{2}\left\{( 1 + \frac { \alpha _ { s } } { 2 \pi } \Delta C _ { q } ^ { N } ) \left[\delta q\left(N, Q^{2}\right)\right.\right. \\
& \left.\left.\quad+\delta \bar{q}\left(N, Q^{2}\right)\right]+\frac{\alpha_{s}}{2 \pi} 2 \Delta C_{g}^{N} \delta g\left(N, Q^{2}\right)\right\} \tag{5}
\end{align*}
$$

In Eq. 5 above, $\delta q\left(N, Q^{2}\right)$ is the quark helicity distribution for quarks of flavor $q$. Correspondingly, $\delta \bar{q}\left(N, Q^{2}\right)$ is the anti-quark helicity distribution. Also in Eq. (5), $\delta q\left(N, Q^{2}\right)=\delta q_{v}\left(N, Q^{2}\right)+\delta \bar{q}\left(N, Q^{2}\right), \delta \bar{q}\left(N, Q^{2}\right)$ and $\delta g\left(N, Q^{2}\right)$ are moments of the polarized parton distributions in a proton. $\Delta C_{q}^{N}$ and $\Delta C_{g}^{N}$ are the $N$-th moments of spin-dependent Wilson coefficients given by

$$
\begin{align*}
\Delta C_{q}^{N}= & \frac{4}{3}\left[-S_{2}(N)+\left(S_{1}(N)\right)^{2}+\left(\frac{3}{2}-\frac{1}{N(N+1)}\right)\right. \\
& \left.\times S_{1}(N)+\frac{1}{N^{2}}+\frac{1}{2 N}+\frac{1}{N+1}-\frac{9}{2}\right] \tag{6}
\end{align*}
$$

and

$$
\begin{equation*}
\Delta C_{g}^{N}=\frac{1}{2}\left[-\frac{N-1}{N(N+1)}\left(S_{1}(N)+1\right)-\frac{1}{N^{2}}+\frac{2}{N(N+1)}\right] \tag{7}
\end{equation*}
$$

with $S_{k}(N)$ defined as in Ref. [12].

The centerpiece of our approach is the Jacobi polynomial expansion; this method was developed and applied to a variety of QCD analyses for unpolarized [14-26] and polarized applications [27-30]. In this approach, we expand the structure functions in terms of Jacobi polynomials $\Theta_{m}^{\alpha, \beta}$ :

$$
\begin{equation*}
x g_{1}^{N_{\max }}\left(x, Q^{2}\right)=x^{\beta}(1-x)^{\alpha} \sum_{n=0}^{N_{\max }} a_{n}\left(Q^{2}\right) \Theta_{n}^{\alpha, \beta}(x) \tag{8}
\end{equation*}
$$

with

$$
\begin{equation*}
a_{n}\left(Q^{2}\right)=\sum_{j=0}^{n} c_{j}^{(n)}(\alpha, \beta) \mathbf{M}\left[x g_{1}\right](j+2) \tag{9}
\end{equation*}
$$

This relates the $g_{1}^{p, n}\left(x, Q^{2}\right)$ structure function with their moments [28]. Obviously in Eq.(9), the $Q^{2}$-dependence of the polarized structure function is defined by the $Q^{2}$ dependence of the moments. In this analysis we use $N_{\max }=9, \alpha=3.0$ and $\beta=0.5$.

The spin-dependent structure functions for the deuteron in Mellin- N space can be decomposed as follows:

$$
\begin{equation*}
g_{1}^{d}\left(N, Q^{2}\right)=\frac{1}{2}\left(1-\frac{3}{2} w_{D}\right)\left[g_{1}^{p}\left(n, Q^{2}\right)+g_{1}^{n}\left(N, Q^{2}\right)\right] \tag{10}
\end{equation*}
$$

where $\omega_{D}=0.05 \pm 0.01$ is the $D$-state wave probability for the deuteron [31]. Using the Mellin-N moments for the proton, neutron and deuteron spin structure functions of Eq. (9), we can perform a fit to extract the unknown parameters.

For the present analysis we use the following data sets: 179 proton data points from EMC[1], HERMES[3, 8], SMC[5], E143[7], E155[4] and COMPASS[2]; 85 neutron data points from E142[11], HERMES[3, 8] and E154[9, 10]; 115 deuteron data points from SMC[5], E143 [7], E155[6] and HERMES[3]. The data sets contain both statistical and systematic errors, and the systematic errors are partly correlated; this leads to an overestimation of the true uncertainty when the statistical and systematic errors are added in quadrature. Additionally, the normalization error is generally specified separately. Using these uncertainties, we fit to an effective $\chi^{2}$ as detailed in Refs. [23, 26]. Additional details are presented in Ref. [27]. In Fig.1, we compare the fit results for the structure functions $g_{1}^{p}\left(x, Q^{2}\right)$ and $g_{1}^{n}\left(x, Q^{2}\right), g_{1}^{d}\left(x, Q^{2}\right)$ at $Q^{2}=5 \mathrm{GeV}^{2}$ with the data, to illustrate the fit quality for the different targets as an example. Furthermore, also the results of the BB [32], GRSV [33], LSS [34], and AAC [35] analyses are shown.


Figure 1: The polarized structure function $x g_{1}^{p, n, d}$ as a function of $x$ in comparison with data from HERMES[3], SMC[5], E142 [11], E143[7], E154[9, 10] and E155 [4]. Also shown are the QCD NLO curves obtained by BB (dashed) [32], GRSV (dashed-dotted) [33], LSS (dashed-dotted-dotted) [34], and AAC (dashed-dashed-dotted) [35] for comparison.

## 3. Nonsinglet spin-dependent structure function

Having investigated the proton, neutron and deuteron spin structure functions, we now turn to the nonsinglet spin-dependent structure function: [3]

$$
\begin{align*}
x g_{1}^{N S}\left(x, Q^{2}\right) & \equiv x g_{1}^{p}\left(x, Q^{2}\right)-x g_{1}^{n}\left(x, Q^{2}\right) \\
& =2\left[x g_{1}^{p}\left(x, Q^{2}\right)-\frac{x g_{1}^{d}\left(x, Q^{2}\right)}{1-\frac{3}{2} \omega_{D}}\right] \tag{11}
\end{align*}
$$

In Fig.2, the $x$ dependence of $x g_{1}^{N S}\left(x, Q^{2}\right)$ is presented for different values of $Q^{2}$ and compared with data from HERMES[3], SMC[5], E143[7]. The nonsinglet structure function shows a behavior similar to that of the deuteron and neutron. The HERMES data provide improved constraints on the $x$ dependence of $x g_{1}^{N S}$. As shown, the data are well described within the errors by our analysis.

The integrals for $g_{1}^{p}, g_{1}^{d}, g_{1}^{n}$ and $g_{1}^{N S}$ calculated at $Q_{0}^{2}=2.5$ and $5 \mathrm{GeV}^{2}$, are given in Table 1 together


Figure 2: The nonsinglet polarized structure function $x g_{1}^{N S}$ as a function of $x$ in comparison with data from HERMES[3], SMC[5], E143[7]. The data are well described by our QCD curves.
with HERMES[3] results. They are computed for $x=$ [0.021, 0.9].

Fig. 3 shows the cumulative integral of $g_{1}^{p}, g_{1}^{n}, g_{1}^{d}$ and $g_{1}^{N S}$ as a function of the lower integration limit $x$, evaluated at $Q^{2}=5 \mathrm{GeV}^{2}$. There is satisfactory agreement between our results and the HERMES[3] data.

## 4. Conclusions

We have performed a QCD analysis of the inclusive polarized DIS charged-lepton-nucleon scattering data at NLO , and extracted the spin structure function $g_{1}\left(x, Q^{2}\right)$ for the proton, neutron, and deuteron. We have used an expansion in Jacobi polynomials to facilitate the analysis, and then defined an effective global $\chi^{2}$ to obtain an acceptable fit [27].

We have also used the above results to construct the nonsinglet spin-dependent structure function $g_{1}^{N S}$, which is in good agreement with the experimental data. As this data is not an input to the fit, this result is evidence of the applicability and universality of the fit.

A FORTRAN package containing the polarized structure functions, as well as the parton densities, can be found in http://particles.ipm.ir/links/QCD.htm.

| $\int g_{1} d x$ | HERMES | MODEL |
| :---: | :---: | :---: |
| $Q^{2}=2.5 \mathrm{GeV}^{2}$ |  |  |
| p | 0.1201 | 0.1179 |
| n | -0.0276 | -0.0292 |
| d | 0.0428 | 0.04045 |
| NS | 0.1477 | 0.1472 |
| $Q^{2}=5 \mathrm{GeV}^{2}$ |  |  |
| p | 0.1211 | 0.1200 |
| n | -0.0268 | -0.0289 |
| d | 0.0436 | 0.0416 |
| NS | 0.1479 | 0.1490 |

Table 1: The integrals for $g_{1}^{p}, g_{1}^{d}, g_{1}^{n}$ and $g_{1}^{N S}$, at $Q_{0}^{2}=2.5$ and $5 \mathrm{GeV}^{2}$ together with HERMES[3] results computed for $x=[0.021,0.9]$.


Figure 3: The value of $\int_{x}^{0.9} g_{1} d x$ for $0.021 \leq x \leq 0.9$ as a function of the lower limit $(x)$ of integration, evaluated at $Q^{2}=5 \mathrm{GeV}^{2}$.

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# Strange quark parton distribution functions and implications for Drell-Yan boson production at the LHC 

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#### Abstract

Global analyses of parton distribution functions (PDFs) have provided incisive constraints on the up and down quark components of the proton, but constraining the other flavor degrees of freedom is more challenging. Higher-order theory predictions and new data sets have contributed to recent improvements. Despite these efforts, the strange quark parton distribution function has a sizable uncertainty, particularly in the small $x$ region. We examine the constraints from experiment and theory, and investigate the impact of this uncertainty on LHC observables. In particular, we study $W / Z$ production to see how the $s$ quark uncertainty propagates to these observables, and examine the extent to which precise measurements at the LHC can provide additional information on the proton flavor structure.


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## I. INTRODUCTION

## A. Motivation

Parton distribution functions (PDFs) provide the essential link between the theoretically calculated partonic cross sections, and the experimentally measured physical cross sections involving hadrons and mesons. This link is crucial if we are to make incisive tests of the standard model (SM), and search for subtle deviations which might signal new physics.

Recent measurements of charm production in neutrino deeply inelastic scattering (DIS), visible as dimuon final states, provide important new information on the strange quark distribution, $s(x)$, of the nucleon [1-16]. We show that despite these recent advances in both the precision data and theoretical predictions, the relative uncertainty on the heavier flavors remains large. We will focus on the strange quark and show the impact of these uncertainties on selected LHC processes.

The production of $W / Z$ bosons is one of the "benchmark" processes used to calibrate our searches for the Higgs boson and other "new physics" signals. We will examine how the uncertainty of the strange quark PDF influences these measurements, and assess how these uncertainties might be reduced.

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## B. Outline

The outline of the presentation is as follows. In Sec. II, we examine the experimental signatures that constrain the strange quark parton distribution. In Sec. III we consider the impact of $s$ quark PDF uncertainties on $W / Z$ production at the LHC, and in Sec. IV we summarize our results. Additional details on PDF fits to dimuon data at next-to-leading order (NLO) are provided in the Appendix.

## II. CONSTRAINING THE PDF FLAVOR COMPONENTS

## A. Extracting the strange quark PDF

In previous global analyses, the predominant information on the strange quark PDF $s(x)$ came from the difference of (large) inclusive cross sections for neutral and charged current DIS. For example, at leading order (LO) in the parton model one finds that the difference between the neutral current (NC) and charged current (CC) DIS $F_{2}$ structure function is proportional to the strange PDF. Specifically if we neglect the charm PDF and isospinviolating terms, we have [17]

$$
\begin{equation*}
\Delta F_{2}=\frac{5}{18} F_{2}^{\mathrm{CC}}-F_{2}^{\mathrm{NC}} \sim \frac{x}{6}[s(x)+\bar{s}(x)] . \tag{1}
\end{equation*}
$$

Because the strange distributions are small compared to the large up and down PDFs, the $s(x)$ extracted from this measurement has large uncertainties. Lacking better information, it was commonly assumed the distribution was of the form

$$
\begin{equation*}
s(x)=\bar{s}(x) \sim \kappa[\bar{u}(x)+\bar{d}(x)] / 2 \tag{2}
\end{equation*}
$$

with $\kappa \sim 1 / 2$.


FIG. 1 (color online). Relative uncertainty of the strange quark PDF as a function of $x$ for $Q=2 \mathrm{GeV}$. The inner band is for the CTEQ6.1 PDF set, and the outer band is for the CTEQ6.6 PDF set. The band is computed as the envelope of $s_{i}(x) / s_{0}(x)$ where $s_{0}(x)$ is the central PDF for each set; for CTEQ6.1, $i=[1,40]$, and for CTEQ6.6, $i=[1,44]$.

This approach was used, for example, in the CTEQ6.1 PDFs [18]. In Fig. 1 we show the relative uncertainty band of the strange quark PDF for the 40 CTEQ6.1 PDF error sets relative to the central value. We observe that over much of the $x$ range the relative uncertainty on the strange PDF is $\leq 5 \%$. The relation of Eq. (2) tells us that this uncertainty band in fact reflects the uncertainty on the up and down sea which is well constrained by DIS measurements; this does not reflect the true uncertainty of $s(x)$.

Beginning with CTEQ6.6 PDFs [19] the neutrinonucleon dimuon data were included in the global fits to more directly constrain the strange quark; thus, Eq. (2) was not used, and two additional fitting parameters were introduced to allow the strange quark to vary independently of the up and down sea. We also display the relative uncertainty band for the CTEQ6.6 PDF set in Fig. 1. We now observe that the relative error on the strange quark is much larger than for the CTEQ6.1 set, particularly for $x<0.01$ where the neutrino-nucleon dimuon data do not provide any constraints. We expect this is a more accurate representation of the true uncertainty.

This general behavior is also exhibited in other global PDF sets with errors [20-23]. For example, the NNPDF Collaboration uses a parametrization-free method for extracting the PDFs; it observes a large increase in the $s(x)$ uncertainty in the small $x$ region which is beyond the constraints of the $\nu$-DIS experiments. (Cf., in particular, Fig. 13 of Ref [21].)

Thus, there is general agreement that the strange quark PDF is poorly constrained, particularly in the small $x$ region.

## B. Constraints from CCFR and NuTeV

The primary source of information on the strange quark at present comes from high-statistics neutrino-nucleon DIS measurements; in particular, the CCFR and NuTeV dimuon experiments have been used to determine the strange

TABLE I. We display the $\chi^{2} / \mathrm{DoF}$ for selected data sets using the CTEQ6M PDF set [12], and a variant of this (labeled "free") which allows for a modified strange quark PDF to accommodate the neutrino dimuon data.

| $\chi^{2} /$ DoF | CTEQ6M | Free |
| :--- | :---: | :---: |
| CCFR $\nu$ dimuon | 1.02 | 0.72 |
| CCFR $\bar{\nu}$ dimuon | 0.58 | 0.59 |
| NuTeV $\nu$ dimuon | 1.81 | 1.44 |
| NuTeV $\bar{\nu}$ dimuon | 1.48 | 1.13 |
| BCDMS $F_{2}^{p}$ | 1.11 | 1.11 |
| BCDMS $F_{2}^{d}$ | 1.10 | 1.11 |
| H1 96/97 | 0.94 | 0.94 |
| H1 98/99 | 1.02 | 1.03 |
| ZEUS 96/97 | 1.14 | 1.15 |
| NMC $F_{2}^{p}$ | 1.52 | 1.49 |
| NMC $F_{2}^{d} / F_{2}^{p}$ | 0.91 | 0.91 |
| CCFR $F_{2}$ | 1.70 | 1.88 |
| CCFR $F_{3}$ | 0.42 | 0.42 |
| E605 | 0.82 | 0.83 |
| NA51 | 0.62 | 0.52 |
| CDF $\ell$ asymmetry | 0.82 | 0.82 |
| E866 | 0.39 | 0.38 |
| D0 jets | 0.71 | 0.67 |
| CDF jets | 1.48 | 1.47 |
| Total $\chi^{2}$ | 2173 | 2133 |

quark PDF with improved accuracy $[6,8,9,16,24-26]$. Neutrino-induced dimuon production $\left(\nu N \rightarrow \mu^{+} \mu^{-} X\right)$ proceeds primarily through the Cabibbo favored $s \rightarrow c$ or $\bar{s} \rightarrow \bar{c}$ subprocess. Hence, this provides information on $s$ and $\bar{s}$ directly; this is in contrast to $\Delta F_{2}$ of Eq. (1). CCFR has $5030 \nu$ and $1060 \bar{\nu}$ dimuon events, and NuTeV has $5012 \nu$ and $1458 \bar{\nu}$ dimuon events, and these cover the approximate range $x \sim[0.01,0.4]$. Additionally, NuTeV used a sign-selected beam to separate the $\nu$ and $\bar{\nu}$ events in order to separately extract $s(x)$ and $\bar{s}(x)$.

## 1. Constraints on $s+\bar{s}$

In Table I we illustrate how the bulk of the data used in the global fits are relatively insensitive to the strange quark distribution. The first column (labeled "CTEQ6M") lists the $\chi^{2} /$ DoF for a variety of data sets used in the CTEQ6M fit [12]. We have also shown the CCFR and NuTeV dimuon data sets in the table, but these were not used in the CTEQ6M fit. The second column (labeled "free") lists results of refitting all the data-including the dimuon data-with a flexible strange quark PDF instead of imposing the relation of Eq. (2); this allows the strange quark PDF to accommodate the dimuon data. Comparing the two columns, we observe that the change of the strange PDF allowed for a greatly improved fit of the dimuon data, while the other data sets are virtually insensitive to this change. ${ }^{1}$

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FIG. 2 (color online). We plot $\chi^{2} / \chi_{0}^{2}$ for the dimuon and the inclusive I data sets evaluated as a function of the strange asymmetry $\left[S^{-}\right] \times 10^{4}$. The fits are denoted with $\square$ for the dimuons and $\boldsymbol{\Delta}$ for inclusive I. Quadratic approximations to the fits are displayed by the solid (red) line for the dimuons and the dashed (green) line for inclusive I.

This exercise demonstrates that most of the data sets of the global analysis are insensitive to the details of the strange quark PDF.

## 2. Constraints on $s-\bar{s}$

The dimuon data can also provide information on the $s(x)$ and $\bar{s}(x)$ quark PDFs separately. In Fig. 2 we display the relative $\chi^{2}$ for the dimuon and "inclusive I" data sets as a function of the strange asymmetry $\left[S^{-}\right]$, where

$$
\begin{equation*}
\left[S^{-}\right] \equiv \int_{0}^{1} x[s(x)-\bar{s}(x)] d x \tag{3}
\end{equation*}
$$

The inclusive I data sets (cf. Ref. [27]) contain the data that are sensitive to $\left[S^{-}\right]$; specifically, the data sets are (a) the neutrino $x F_{3}$ data from CCFR and CDHSW as neutrino $x F_{3}$ is proportional to the difference of quark and antiquark PDFs, and (b) the CDF $W$-asymmetry measurement which can receive contributions from the $s g \rightarrow W c$ subprocess. Figure 2 clearly shows that the dimuon data provide the strongest constraints on the strange asymmetry $\left[S^{-}\right]$.

## C. HERMES

The HERMES experiment measured the strange PDF via charged kaon production in positron-deuteron DIS [28]; these results are displayed in Fig. 3. For comparison, the strange quark and total sea distributions from CTEQ6L are also plotted.


FIG. 3 (color online). The strange parton distribution $x S(x)=$ $x[s(x)+\bar{s}(x)]$ from the measured Hermes multiplicity for charged kaons evolved to $Q^{2}=2.5 \mathrm{GeV}^{2}$. The dotted green curve is a Hermes 3-parameter fit: $S(x)=x^{-0.924} e^{-x / 0.0404}(1-$ $x$ ), the dashed blue curve is the sum of light antiquarks $x(\bar{u}+\bar{d})$ from CTEQ6L, the dash-dotted blue curve is $x S(x)$ from CTEQ6L, and the solid red curve is the $x S(x)$ from CTEQ6.6. Hermes data points and fit are from Ref. [28].

The HERMES data suggest that the $x$ dependence of the strange quark distribution is quite different from the form assumed for the CTEQ6 set. In particular, HERMES obtains a strange quark distribution that is suppressed in the region $x \gtrsim 0.1$ but then grows quickly for $x<0.1$ and exceeds the CTEQ6L value in the small $x$ region by more than a factor of 2 .

To gauge the compatibility of this result with the displayed PDFs, we can replace the initial $s(x)$ distribution with the form preferred by HERMES, and then evaluate the shift of the $\chi^{2}$ with this additional constraint. A preliminary investigation with this procedure indicates that the HERMES $s(x)$ distribution could strongly influence two data sets of the global fits. The first set is the neutrinonucleon dimuon data which control $s(x)$ in the intermediate $x$ region. The second set is the HERA measurement of $F_{2}$ in the small $x$ region where the statistical errors are particularly small.

In Fig. 3 we also show $x S(x)$ from CTEQ6.6; while the HERMES data are below the CTEQ6.6 result in the $x \sim 0.1$ region, they agree quite well at both the higher and lower $x$ values.

While these comparisons are sufficient to gauge the general influence of the Hermes result, a complete analysis that includes the Hermes data dynamically in the global fit is required to draw quantitative conclusions.

## D. CHORUS

The CHORUS experiment [29-31] measured the neutrino structure functions $F_{2}, x F_{3}, R$ in collisions of signselected neutrinos and antineutrinos with a lead target (lead-scintillator CHORUS calorimeter) in the CERN Super Proton Synchrotron (SPS) neutrino beam line. The
experiment collected over $3 \mathrm{M} \nu_{\mu}$ and $1 \mathrm{M} \bar{\nu}_{\mu}$ charged current events in the kinematic range $0.01<x<0.7$, $0.05<y<0.95,10<E_{\nu}<100$.

These data were analyzed in the context of a global fit in Ref. [32] which was based on the CTEQ6.1 PDFs. This analysis made use of the correlated systematic errors and found that the CHORUS data are generally compatible with the other data sets, including the NuTeV data. Thus, the CHORUS data are consistent with the strange distribution extracted in CTEQ6.1.

## E. NOMAD

The NOMAD experiment measured neutrino-induced charm dimuon production to directly probe the $s$ quark PDF [33-35]. Protons from the CERN SPS synchrotron ( 450 GeV ) struck a beryllium target to produce a neutrino beam with a mean energy of 27 GeV . NOMAD used an ironscintillator hadronic calorimeter to collect a very high statistics ( 15 K ) neutrino-induced charm dimuon sample [34].

Using kinematic cuts of $E_{\mu 1}, E_{\mu 2}>4.5 \mathrm{GeV}, 15<$ $E_{\nu}<300 \mathrm{GeV}$, and $Q^{2}>1 \mathrm{GeV}^{2}$, NOMAD performed a leading-order QCD analysis of 2714 neutrino- and 115 antineutrino-induced opposite sign dimuon events [33]. The ratio of the strange to nonstrange sea in the nucleon was measured to be $\kappa=0.48_{-0.07-0.12}^{+0.09+0.17}$; this is consistent with the values used in the global fits (cf. Fig. 4).

The data analysis is continuing, and it will be very interesting to include this data set into the global fits as the large dimuon statistics have the potential to strongly influence the extracted PDFs.

## F. MINER $\boldsymbol{\nu}$ A

The cross sections in neutrino DIS experiments from NuTeV, CCFR, CHORUS and NOMAD have been mea-


FIG. 4 (color online). $\kappa(x, Q)$ vs $x$ for $Q=1.5 \mathrm{GeV}$ for a selection of PDFs, where $\kappa(x, Q)$ is defined in Eq. (4). The curves (top to bottom) are CTEQ6.6 (solid, red), CTEQ6.5 (dotted, black), and CTEQ6.1 (dashed, purple). The wider (blue) band represents the uncertainty for CTEQ6.6 as computed by Eq. (5), the inner (green) band represents uncertainty given by the envelope of $\kappa(x, Q)$ values obtained with the 44 CTEQ6.6 error sets.
sured using heavy nuclear targets. In order to use these measurements in a global analysis of proton PDFs, these data must be converted to the corresponding proton or isoscalar results [36-42]. For example, the nuclear correction factors used in the CTEQ6 global analysis were extracted from $\ell^{ \pm} N$ DIS processes on a variety of nuclei, and then applied to $\nu N$ DIS on heavy nuclear targets. In a series of recent studies it was found that the $\ell^{ \pm} N$ nuclear correction factors could differ substantially from the optimal $\nu N$ nuclear correction factors [39-43].

Furthermore, the nuclear corrections depend to a certain degree on the specific observable as they contain different combinations of the partons; the nuclear correction factors for dimuon production will not be exactly the same as the ones for the structure function $F_{2}$ or $F_{3}$. The impact of varying the nuclear corrections on the strange quark PDF has to be done in the context of a global analysis which we leave for a future study.

The MINER $\nu$ A experiment has the opportunity to help resolve some of these important questions as it can measure the neutrino DIS cross sections on a variety of light and heavy targets. It uses the NuMI beam line at Fermilab to measure low energy neutrino interactions to study neutrino oscillations and also the strong dynamics of the neutrino-nucleon interactions. MINER $\nu \mathrm{A}$ completed construction in 2010, and it has begun data collection. MINER $\nu$ A can measure neutrino interactions on a variety of targets including plastic, helium, carbon, water, iron, and lead. For $4 \times 10^{20}$ protons on target it can generate over 1 M charged current events on plastic.

These high-statistics data on a variety of nuclear targets could allow us to accurately characterize the nuclear correction factors as a function of the nuclear $A$ from helium to lead. These data will be very useful in resolving questions about the nuclear corrections, and we look forward to the results in the near future.

## G. CDF and DO

At the Tevatron, the CDF [44] and D0 [45] Collaborations measured $W c$ final states in $p \bar{p}$ at $\sqrt{S}=$ 1.96 TeV using the semileptonic decay of the charm and the correlation between the charge of the $W$ and the charm decay. Additionally, a recent study has investigated the impact of the $W+$ dijet cross section on the strange PDF [46]. These measurements are especially valuable for two reasons. First, there are no nuclear correction factors as the initial state is $p$ or $\bar{p}$. Second, this is in a very different kinematic region as compared to the fixed-target neutrino experiments. Thus, these have the potential to constrain the strange quark PDF in a manner complementary to the $\nu N$ DIS measurements; however, the hadron-hadron initial state is challenging. Using approximately $1 \mathrm{fb}^{-1}$ of data, both CDF and D0 find their measurements to be in agreement with theoretical expectations of the standard model. Updated analyses with larger data sets are in progress and it
will be interesting to see the impact of these improved constraints on the strange quark PDF.

## H. Strange quark uncertainty

The combination of the above results underscores the observation that our knowledge of the strange quark is limited. To illustrate this point in another manner, in Fig. 4 we display $\kappa(x, Q)$ for a selection of PDF sets. Here, we define

$$
\begin{equation*}
\kappa(x, Q)=\frac{s(x, Q)}{[\bar{u}(x, Q)+\bar{d}(x, Q)] / 2} \tag{4}
\end{equation*}
$$

which is essentially a differential version of the $\kappa$ parameter of Eq. (2); this allows us to gauge the amount of the strange PDF inside the proton compared to the average up and down sea quark PDFs. If we had exact $S U(3)$ symmetry we would expect $\bar{u}=\bar{d}=\bar{s}$ and $\kappa(x, Q) \sim 1$. As the strange quark is heavier than the up and down quarks, we expect this component to be suppressed relative to the up and down quarks, and we would predict $\bar{u} \simeq \bar{d}>\bar{s}$ which would yield $\kappa(x, Q)<1$. Thus, $\kappa(x, Q)$ is a measure of the $S U(3)$ breaking across the $x$ and $Q$ range.

In Fig. 4 we observe that the CTEQ6.1 and CTEQ6.5 PDF sets have $\kappa(x, Q) \sim 1 / 2$; this was by design as the constraint of Eq. (2) was used to set the initial $s(x)$ distribution. The exception is CTEQ6.6 which did not impose Eq. (2); we observe that this set has $\kappa(x, Q) \sim 1 / 2$ for $x \sim 0.1$ (where the dimuon DIS data have smaller uncertainties), but is a factor of 2 larger than the other PDF sets for small $x$ values. In Fig. 4 we also show the uncertainty on $s(x)$ computed as [12]

$$
\begin{equation*}
\Delta X=\frac{1}{2} \sqrt{\sum_{i=1}^{N_{p}}\left[X\left(S_{i}^{+}\right)-X\left(S_{i}^{-}\right)\right]^{2}}, \tag{5}
\end{equation*}
$$

which is shown as a wider (blue) band; ${ }^{2}$ this results in a band which is larger than simply taking the spread of the 44 CTEQ6.6 error PDFs [inner (green) band].

In order to show the effect of the Dokshitzer, Gribov, Lipatov, Altarelli, Parisi evolution on the strange distribution, we display $\kappa(x, Q)$ for CTEQ6.1 and CTEQ6.6 at both a low and high $Q$ scale in Fig. 5. As we explore higher scales, the production of $s(x)$ by gluon splitting moves $\kappa(x, Q)$ toward the $S U(3)$-symmetric limit. This trend is especially pronounced at low $x$ values. Thus, as the LHC $W / Z$ production is centered in the range $x \sim 0.01$, we will be particularly interested in the $\kappa(x, Q)$ changes in this region.

These results reflect the relevant $x$ range of the constraints on the strange quark PDF, and how they depend on the $Q$ scale. In the next section we will investigate the

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FIG. 5 (color online). $\kappa(x, Q)$ vs $x$ showing the evolution from low to high scales. The solid (red) lines are for CTEQ6.6, and the dashed (purple) lines are for CTEQ6.1. The lower pair of lines (red and purple) are for $Q=1.5 \mathrm{GeV}$ and the upper for $Q=80 \mathrm{GeV}$.
implications of this uncertainty on the Drell-Yan $W / Z$ boson production at the LHC.

## III. IMPLICATIONS FOR DRELL-YAN $W / Z$ PRODUCTION AT THE LHC

The Drell-Yan production of $W^{ \pm}$and $Z$ bosons at hadron colliders can provide precise measurements for electroweak observables such as the $W$ boson mass $[47,48]$ and width, the weak mixing angle in $\gamma^{*} / Z$ production [49], and the lepton asymmetry in $W$ production. These results can measure fundamental parameters of the standard model and constrain the Higgs boson mass. If a Higgs boson is found at the LHC, Drell-Yan $W / Z$ boson production will help in the search for deviations of the SM and to reveal new physics signals [50-52]. For instance, new heavy gauge bosons could be discovered in the invariant lepton distribution, or new particles and interactions might leave a footprint in the Peskin-Takeuchi $S$ and $T$ parameters [53].

Furthermore, the $W$ and $Z$ boson cross section benchmark processes are intended to be used for detector calibration and luminosity monitoring [54]; to perform these tasks it is essential that we know the impact of the PDF uncertainties on these measurements. The impact on these benchmark processes, and the Higgs boson production, were studied in Refs. [55-57]. In the following, we will investigate the influence of the PDFs on the rapidity distributions of the Drell-Yan production process. Conversely, it may be possible to use the $W / Z$ production process to further constrain the parton distribution functions in general, and the strange quark PDF, in particular. As noted in Ref. [49], when looking for new physics signals it is important not to mix the information used to constrain the PDFs and the new physics as this would lead to circular reasoning.

As we move from the Tevatron to the LHC scattering processes, the kinematics of the incoming partons changes
considerably; in Fig. 6 we show the momentum fractions $x_{A}$ and $x_{B}$ of the incoming parton $A$ and parton $B$ for the Tevatron Run-2 $(\sqrt{S}=1.96 \mathrm{TeV})$ and the LHC with $\sqrt{S}=$ 7 TeV and $\sqrt{S}=14 \mathrm{TeV}$. The solid (red) lines show the range of $x_{A}$ and $x_{B}$ probed by $W^{ \pm}$and $Z$ boson production. At the Tevatron, values of $x_{A, B}$ down to $2 \times 10^{-3}$ are probed for large rapidities of $y_{W / Z}=3$. However, at the LHC much smaller values of $x_{A}$ and $x_{B}$ become important due to the larger CMS energy and broader rapidity span. For $\sqrt{S}=7 \mathrm{TeV}$, the PDFs are probed for $x$ values as small as $2 \times 10^{-4}$ for rapidities up to $\sim 4.5$. With $\sqrt{S}=$ 14 TeV , even larger rapidities of $y \sim 5$ and smaller values of $x_{A / B}$ of $4 \times 10^{-5}$ might be reached.

## A. LHC measurements

The importance of the PDF uncertainties to the LHC measurements was already evident in the 2010 and preliminary 2011 data.

ATLAS presented measurements of the Drell-Yan $W / Z$ production at the $\sqrt{S}=7 \mathrm{TeV}$ with $35 \mathrm{pb}^{-1}$ [58]. These results include not only the measurement of total cross section and transverse distributions, but also a first measurement of the rapidity distributions for $Z \rightarrow l^{+} l^{-}$as well as $W^{+} \rightarrow l^{+} \nu_{l}$ and $W^{-} \rightarrow l^{-} \bar{\nu}_{l}$. Additionally, ATLAS has used $W / Z$ production to infer constraints on the strange quark distribution, and it measures $r_{s}=0.5(s+\bar{s}) / \bar{d}=$ $1.00_{-0.28}^{+0.25}$ at $Q^{2}=1.9 \mathrm{GeV}^{2}$ and $x=0.023$ [59].


FIG. 6 (color online). Parton momentum fractions $x_{A}$ and $x_{B}$ accessible in $W$ and $Z$ boson production in the Tevatron Run-2 ( $\sqrt{S}=1.96 \mathrm{TeV}$ ), and at the LHC $(\sqrt{S}=\{7,14\} \mathrm{TeV})$. The accessible ranges of $x_{A}$ and $x_{B}$ are shown by the solid lines. The contours of the constant rapidity $y$ are shown by the inclined dotted lines.

CMS has measured the rapidity and transverse momentum distributions for $Z \rightarrow l^{+} l^{-}$production [60] and inclusive $W / Z$ production [61] using $36 \mathrm{pb}^{-1}$ of data. Additionally CMS has measured the weak mixing angle [49], the forward-backward asymmetry in $\gamma^{*} / Z$ production [62], and the lepton charge asymmetry in $W$ production [63,64].

LHCb has measured the $W$ charge asymmetry in Refs. [65,66]. These measurements show, already with these data samples, the PDF uncertainties are important and can be the leading source of measurement uncertainty.

Additionally, CMS has analyzed $W+c$ production which is directly sensitive to the $s$ and $\bar{s}$ contribution of the proton; the results for the $36 \mathrm{pb}^{-1}$ data sample are given in Ref. [67].

## B. Strange contribution to $W / Z$ production

Because the proton-proton LHC has a different initial state and a higher CMS energy than the Tevatron, the relative contributions of the partonic subprocesses of the $W^{ \pm} / Z$ production change significantly. At the LHC, the contributions of the second generation quarks $\{s, c\}$ are greatly enhanced. Additionally, the $W^{+}$and $W^{-}$rapidity distributions are no longer related by a simple $y \rightarrow-y$ reflection symmetry due to the $p p$ initial state. In Fig. 7 we display the contributions from the different partonic cross sections which contribute to $W^{ \pm}$and $Z$ production at LO.

Figure 7(a) shows the rapidity distribution at the Tevatron. For $W^{+}\left(W^{-}\right)$production, the $u \bar{d}(\bar{u} d)$ channel (dotted black lines) contributes $90 \%$ of the cross section, while in $Z$ production the $u \bar{u}$ (dotted black line) and $d \bar{d}$ (dash-dotted black line) subprocesses contribute $93 \%$ of the cross section. The first generation quarks $\{u, d\}$ therefore dominate the production process while contributions from strange quarks [(red) dashed and (blue) dash-dotted lines] are comparably small with $5 \%$ for $W^{ \pm}$and $5 \%(s \bar{s})$ for $Z$ boson production.

At the LHC, subprocesses containing strange quarks are considerably more important as shown in Fig. 7(b) for a CMS energy of 7 TeV and in Fig. 7(c) for 14 TeV . For $W^{-}$ production (left plots), the (blue) dash-dotted lines show the $\bar{u} s$ channel while the (red) dashed lines show the $\bar{c} s$ contribution. At 14 TeV the $\bar{c} s \rightarrow W^{-}$subprocess contributes $28 \%$ to the cross section, while the $\bar{u} s \rightarrow W^{-}$subprocess contributes only $2 \%$ as this is suppressed by the off-diagonal Cabibbo-Kobayashi-Maskawa matrix entry. For $W^{+}$production channels, the $u \bar{s}$ channel [(blue) dash-dotted lines] contributes only $2 \%$, while the $c \bar{s}$ channel [(red) dashed lines] yields $21 \%$. Notice the absolute values of the $\bar{c} s \rightarrow W^{-}$and $c \bar{s} \rightarrow W^{+}$contributions are the same; however, the relative contribution is smaller for $W^{+}$ production due to the larger up quark valence contribution in the $u \bar{d} \rightarrow W^{+}$subprocess as compared to $\bar{u} d \rightarrow W^{-}$.

The rapidity distributions of the total $W^{-}$and $W^{+}$boson production differ markedly at the LHC because of the


FIG. 7 (color online). Partonic contributions to the differential cross section of on-shell $W^{ \pm} / Z$ boson production at LO as a function of the vector boson rapidity. Partonic contributions containing a strange or antistrange quark are denoted by (red) dashed and (blue) dash-dotted lines. The solid lines show the total contribution.
different valence quark contributions from $u$ and $d$. This effect is also present in the $\bar{u} s \rightarrow W^{-}$and $u \bar{s} \rightarrow W^{+}$ [(blue) dash-dotted lines] subprocess. We will comment more on this feature in the following subsection.

Comparing Fig. 7(a) with Fig. 7(c), we note the LHC explores a much larger rapidity range. For channels containing strange quarks, $\left|y_{W / Z}\right|$ can be measured up to $y \approx$ 4.5 at the LHC, compared to $y \approx 2.5$ at the Tevatron; therefore smaller values of $x$ of the strange quark distribution can be probed.

Additionally, as at the Tevatron, we can use $W^{-}$production to probe the strange quark PDF while using $W^{+}$ production to probe the antistrange PDF.

While the LO illustration of Fig. 7 provides a useful guide, in Fig. 8 we display the strange quark contribution to the differential cross section $d^{2} \sigma / d M / d y$ of on-shell $W^{-}$, $W^{+}, Z$ boson production computed at next-to-next-toleading order (NNLO) using the VRAP program [68]. We display the LHC results for $W^{ \pm}$and $Z$ with $\sqrt{S}$ of both 7 TeV and 14 TeV , where the (yellow) band represents
the strange quark initiated contributions to the total differential cross section.

The figures impressively highlight the large contribution of the strange and antistrange quark subprocesses at the LHC. Consequently it is essential to constrain the strange PDF if we are to make accurate predictions and to perform precision measurements. Figure 8 also demonstrates clearly the very different rapidity profiles of the strange quark (arising from the sea distribution) compared to the $u$ and $d$ quark terms which are dominated by the valence distributions. This property is most evident for the case of $W^{+}$production. Here, the dominant $u \bar{d}$ contribution has a twin-peak structure due to the harder valence distribution, while the $c \bar{s}$ distribution has a single peak centered at $y=0$. The total distribution is then a linear combination of the twin-peak and single-peak distributions, and these are weighted by the corresponding PDF.

Therefore, a detailed measurement of the rapidity distribution of the $W^{ \pm} / Z$ bosons can yield information about the contributions of the $s$ quark relative to the $u, d$ quarks.


FIG. 8 (color online). Contribution of the strange quark to $W^{ \pm} / Z$ production at the LHC.

As this is a relative measurement, rather than an absolute cross section measurement, it is reasonable to expect that this could be achieved with high precision once sufficient statistics are collected. Consequently, this is an ideal measurement where the LHC data could lead to stronger constraints on the PDFs.

## C. PDF uncertainty of the $W / Z$ rapidity distributions

To estimate the influence of the PDF uncertainties (and, in particular, the strange quark PDF ) on the $W / Z$ production process and its differential distributions at the LHC, we will use the different PDF sets within CTEQ6.6 as well as compare the sets of different PDF groups.

In Fig. 9(a), we display the differential cross section $d^{2} \sigma / d M / d y$ for $W^{ \pm} / Z$ boson production at the LHC at $\sqrt{S}=7 \mathrm{TeV}$ using the 44 error PDF sets of CTEQ6.6. To better resolve these PDF uncertainties, we plot the ratio of the differential cross section $d^{2} \sigma / d M / d y$ compared to the central value in Fig. 9(b). We observe that the uncertainty due to the PDFs as measured by this band is between $\pm 3 \%$ and $\pm 4 \%$ for central boson rapidities of $-3 \leq y_{W / Z} \leq$ +3 . For larger rapidities, the PDF uncertainties increase dramatically, but the cross section vanishes.

For comparison, in Fig. 9(c) we display the (yellow) band of CTEQ6.6 error PDFs together with the results using other contemporary PDF sets. The (yellow) band shows the span of the 44 CTEQ6.6 error PDFs of Fig. 9(b), and the solid lines show the rapidity distribution from the
selection of PDFs; all have been scaled to the central value for the CETQ6.6 set. ${ }^{3}$ We observe that the choice of PDF sets can result in differences ranging up to $\pm 8 \%$ for $-2 \leq$ $y_{W / Z} \leq+2$ and even up to $\pm 10 \%$ for $-3 \leq\left|y_{W / Z}\right| \leq 3$, which is well beyond the $\pm 3 \%$ and $\pm 4 \%$ range displayed in Fig. 9(b); note the different scales used in Figs. 9(b) and 9(c). However, if we compute the PDF uncertainty band using Eq. (5) as specified by Ref. [12] we find an estimated uncertainty of $\sim 15 \%$ (depending on the rapidity) which generally does encompass the range of PDFs displayed in Fig. 9(c).

While the band of error PDFs provides an efficient method to quantify the uncertainty, the range spanned by the different PDF sets illustrates there are other important factors which must be considered to encompass the full range of possibilities.

## D. Correlations of the $\boldsymbol{W} / \boldsymbol{Z}$ rapidity distributions

The leptonic decay modes of the $W / Z$ bosons provide a powerful tool for precision measurements of electroweak parameters such as the $W$ boson mass. As the leptonic

[^107]
(a) $d^{2} \sigma / d M / d y$ in $\mathrm{pb} / \mathrm{GeV}$ for $p p \rightarrow W^{-}+X$ (left), $p p \rightarrow W^{+}+X$ (middle), and $p p \rightarrow Z, \gamma^{*}+X$ (right) production at the LHC for 7 TeV with CTEQ6.6 using the VRAP program [68] at NNLO.

(c) $d^{2} \sigma / d M / d y$ for $\left\{W^{-}, W^{+}, Z\right\}$ production at the LHC for $\sqrt{S}=7 \mathrm{TeV}$ with a selection of PDFs using the VRAP program at NNLO. The (yellow) band is for the CTEQ6.6 set [19], and the other curves are for the central values of different PDF sets (see $t e x t)$. All plots are scaled by the central value for the CETQ6.6 set. Note the scale of this figure is larger than for Fig. 9 b .

FIG. 9 (color online). PDF uncertainty bands for on-shell $W^{-}$(left plots), $W^{+}$(middle plots), and $Z$ (right plots) production at the LHC for $\sqrt{S}=7 \mathrm{TeV}$.
decay of the $W$ boson contains a neutrino ( $W \rightarrow \ell \nu$ ), this process must be modeled to account for the missing neutrino. The $W$ mass can then be measured by studying the transverse momentum distribution of the decay lepton $\ell$ or the transverse mass of the $\ell \nu$ pair. Performing this measurement, the Drell-Yan $Z$ boson production process is used to calibrate the leptonic $W$ process because the $Z$ can decay into two visible leptons $Z \rightarrow \ell^{+} \ell^{-}$. This method works to the extent that the production processes of the $W$ and $Z$ bosons are correlated.

One possible measure to gauge the correlation of the PDF uncertainty is the ratio of the $W$ and $Z$ boson differential cross section. We compute $d^{2} \sigma / d M / d y$ for $W^{ \pm}$ compared to $Z$, and divide by the central PDF results to see the uncertainty band on a relative scale. Schematically we define

$$
\begin{equation*}
R^{ \pm}=\left[\frac{d \sigma\left(W^{ \pm}\right)}{d \sigma(Z)}\right] /\left[\frac{d \sigma\left(W^{ \pm}\right)}{d \sigma(Z)}\right]_{0}, \tag{6}
\end{equation*}
$$

where the " 0 " subscript denotes the "central" PDF set. The resulting distributions are displayed in Fig. 10(a) for $W^{-}$production and in Fig. 10(b) for $W^{+}$production. The left plot in each figure shows the distributions for the CTEQ6.5 PDF set, and the right plot the distributions for CTEQ6.6. We observe that the uncertainty band is generally $\pm 1 \%$ for central rapidities of $-2 \leq y_{W / Z}<+2$; this is smaller than in the previous case, where the absolute uncertainty was investigated. For larger rapidity ( $\left|y_{W / Z}\right|>2$ ) the uncertainty band exceeds the $\pm 1 \%$ range of the plot.

In Fig. 10, we plot the sum of the differential $W^{+}$and $W^{-}$cross sections with respect to the differential $Z$ boson


FIG. 10 (color online). Ratios of the differential $W^{ \pm}$and $Z$ production cross section as defined in Eqs. (6) and (7) at the LHC for $\sqrt{S}=7 \mathrm{TeV}$.
cross section, again normalized to the distribution of the central PDF set. We define

$$
\begin{equation*}
R=\left[\frac{d \sigma\left(W^{+}+W^{-}\right)}{d \sigma(Z)}\right] /\left[\frac{d \sigma\left(W^{+}+W^{-}\right)}{d \sigma(Z)}\right]_{0} \tag{7}
\end{equation*}
$$

for both the CTEQ6.5 and CTEQ6.6 PDFs.
The contrast in Fig. 10(c) is striking. For the CTEQ6.5 PDFs, we observe that $W^{ \pm}$and $Z$ processes are strongly correlated, while for the CTEQ6.6 the spread of the PDF band is substantially larger. For example, the double ratio for CTEQ6.5 has a spread of approximately $\pm 0.2 \%$ within the central rapidity range of $-3 \leq y_{W / Z} \leq+3$, while the uncertainty for CTEQ6.6 is much wider in this rapidity region.

The primary difference that is driving this result is the different strange PDF. For CTEQ6.5 the strange quark was
defined by Eq. (2) while CTEQ6.6 introduced two extra fitting parameters which allowed the strange PDF to vary independently from the up and down sea. Thus, the uncertainty of the CTEQ6.6 distributions more accurately reflects the true uncertainty.

Another means to see how the additional freedom of the strange quark introduces a decorrelation of the $W^{ \pm}$and $Z$ processes is evident in Fig. 11 which displays the correlation of the $W^{ \pm}$and $Z$ boson cross sections for a selection of CTEQ PDFs. Except for CTEQ6.6, all the PDFs make use of Eq. (2) and yield results that lie along a straight line in the $\left\{\sigma_{W}, \sigma_{Z}\right\}$ plane. Because CTEQ6.6 does not use Eq. (2), the freedom of the strange quark PDF is reflected in the freedom of the $W^{ \pm}$and $Z$ cross sections values.

The above examples demonstrate the subtle features inherent in evaluating the PDF uncertainties. For precision measurements it is important to better constrain the parton


FIG. 11 (color online). Correlation of the $W^{ \pm}$and $Z$ cross sections for a selection of PDF sets. Figure taken from Ref. [19].
distributions at the LHC, in particular, the strange and antistrange quark PDFs.

## IV. CONCLUSION

We have investigated the constraints of the strange and antistrange PDFs and their impact on the Drell-Yan $W / Z$ boson production at the LHC.

Specifically, we observe that the strange quark is rather poorly constrained, particularly in the low $x$ region which is sensitive to $W / Z$ production at the LHC. Improved analyses from neutrino DIS measurements could help reduce this uncertainty. Conversely, precision measurements of $W / Z$ production at the LHC may provide input to the global PDF analyses which could further constrain these distributions.

In particular, the rapidity distribution of the $W / Z$ bosons provides an incisive measure of the mix of valence and sea quarks, and the prospect of measuring this at the LHC in the near future is excellent.

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## APPENDIX: PDF FITS WITH THE DIMUON DATA

We have repeated the LO analysis of Ref. [27] and extended this using the NLO calculation for dimuon production $[74,75]$. We have performed a series of fits to the data which includes the dimuon data. The results of the $\left\{A, B^{+}, B, B^{-}, C\right\}$ fits ${ }^{4}$ using the LO dimuon analysis are shown in Table II, and those with the NLO analysis are in Table III. The fits are sorted left-to-right by the integrated strange quark asymmetry $\left[S^{-}\right]$(scaled by $10^{4}$ ). The cells display the $\chi^{2}$ relative to $\chi_{0}^{2}$ for the indicated data set where we choose $\chi_{0}^{2}$ to be the $\chi^{2}$ value from the LO- $B$ fit; this allows us to compare the incremental changes as we shift [ $S^{-}$] and alter the constraints. The values in parentheses are the $\chi^{2} / \mathrm{DoF}$ for each data subset. The $B$ fit is the overall best fit to the data. The $B^{+}$and $B^{-}$sets modify the $B$ fit using the Lagrange multiplier method to determine the ranges of the $\left[S^{-}\right.$] parameter defined in Eq. (3).

For example, the LO $B^{+}$fit demonstrates that we can increase $\left[S^{-}\right.$] from 15.98 to 54.85 , but the dimuon $\chi^{2}$ increases by $33 / 174 \sim 21 \%$ while the overall $\chi^{2}$ increases by only $39 / 2465 \sim 2 \%$; thus, the shift of [ $S^{-}$] is strongly constrained by the dimuon data, and the remaining data are relatively insensitive to this quantity.

Comparing the NLO- $B$ fit to the LO- $B$ fit we note that $\chi^{2} /$ DoF has decreased both for the dimuon set and the entire data set; while this decrease is not dramatic, it is encouraging to see that the proper NLO treatment of the data results in an improved fit. As before, we observe that for the NLO $B^{+}$fit, we can increase $\left[S^{-}\right.$] from 13.72 to 63.75, but the dimuon $\chi^{2}$ increases by $92 / 174 \sim 53 \%$ while the overall $\chi^{2}$ increases by only $106 / 2465 \sim 4 \%$; again, the shift of $\left[S^{-}\right]$is primarily constrained by the dimuon data.

In Fig. 2 we have plotted the ratio $\chi^{2} / \chi_{0}^{2}$ for the individual dimuon and inclusive I data sets [27] evaluated

[^108]TABLE II. Fit results using the LO dimuon calculation. We present the integrated strange quark asymmetry [ $S^{-}$], and the cells display $\chi^{2} / \chi_{0}^{2}$, and the values in parentheses are the $\chi^{2} /$ DoF for each data subset. Note $\chi_{0}^{2}$ is calibrated from the LO $B$ fit.

| LO dimuon | Number of points | $B^{+}$ | $A$ | $B$ | $C$ | $B^{-}$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| $\left[S^{-}\right] \times 10^{4}$ | $\ldots$ | 54.85 | 31.18 | 15.98 | 10.32 | -17.72 |
| Entire data | 2465 | $1.015(1.100)$ | $1.001(1.085)$ | $1.000(1.084)$ | $1.002(1.086)$ | $1.018(1.103)$ |
| Dimuon | 174 | $1.289(0.941)$ | $1.018(0.743)$ | $1.000(0.730)$ | $0.996(0.727)$ | $1.241(0.906)$ |
| Inclusive I | 194 | $0.978(0.711)$ | $0.961(0.699)$ | $1.000(0.727)$ | $1.029(0.748)$ | $1.085(0.789)$ |
| Dimuon + I | 368 | $1.126(0.820)$ | $0.989(0.720)$ | $1.000(0.728)$ | $1.014(0.738)$ | $1.160(0.844)$ |
| Inclusive II | 2097 | $1.012(1.120)$ | $1.014(1.123)$ | $1.000(1.107)$ | $1.011(1.119)$ | $1.011(1.119)$ |

TABLE III. Fit results using the NLO dimuon calculation. We present the integrated strange quark asymmetry [ $S^{-}$], and the cells display $\chi^{2} / \chi_{0}^{2}$, and the values in parentheses are the $\chi^{2} / \mathrm{DoF}$ for each data subset.

| NLO dimuon | Number of points | $B^{+}$ | $A$ | $B$ | $C$ | $B^{-}$ |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| $\left[S^{-}\right] \times 10^{4}$ | $\ldots$ | 63.75 | 23.92 | 13.72 | 12.81 | -18.59 |
| Entire data | 2465 | $1.033(1.120)$ | $0.995(1.079)$ | $0.994(1.077)$ | $0.994(1.077)$ | $1.025(1.111)$ |
| Dimuon | 174 | $1.660(1.212)$ | $0.960(0.701)$ | $0.936(0.683)$ | $0.937(0.684)$ | $1.416(1.034)$ |
| Inclusive I | 194 | $0.977(0.710)$ | $0.974(0.708)$ | $1.008(0.733)$ | $1.017(0.739)$ | $1.088(0.791)$ |
| Dimuon + I | 368 | $1.301(0.947)$ | $0.968(0.705)$ | $0.974(0.709)$ | $0.979(0.713)$ | $1.245(0.906)$ |
| Inclusive II | 2097 | $1.012(1.120)$ | $1.009(1.117)$ | $1.007(1.115)$ | $1.005(1.113)$ | $1.010(1.118)$ |

for a series of NLO $B$ fits as a function of the strange asymmetry $\left[S^{-}\right] \times 10^{4}$. This plot allows us to see the contribution of each data set as we shift the strange asymmetry. Again the inclusive I data sets are essentially
unchanged as the treatment of the dimuons only affects these data indirectly. As before, this data set is mildly sensitive to the dimuons, and weakly prefers larger values of $\left[S^{-}\right.$.
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# Heavy Quarks: lessons learned from HERA and Tevatron 

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#### Abstract

We review some of the recent developments which have enabled the heavy quark mass to be incorporated into both the calculation of the hard-scattering cross section and the PDFs. We compare and contrast some of the schemes that have been used in recent global PDF analyses, and look at issues that arise when these calculations are extended to NNLO.


## 1. Introduction

The production of heavy quarks in high energy processes has become an increasingly important subject of study both theoretically and experimentally. The theory of heavy quark production in perturbative Quantum Chromodynamics (PQCD) is more challenging than that of light parton (jet) production because of the new physics issues brought about by the additional heavy quark mass scale. The correct theory must properly take into account the changing role of the heavy quark over the full kinematic range of the relevant process from the threshold region (where the quark behaves like a typical "heavy particle") to the asymptotic region (where the same quark behaves effectively like a parton, similar to the well known light quarks $\{u, d, s\}$ ).

We review theoretical methods which have been advanced to improve existing QCD calculations of heavy quark production, and the impact on recent experimental results from HERA and the Tevatron.

The ACOT renormalization scheme provides a mechanism to incorporate the heavy quark mass into the theoretical calculation of heavy quark production both kinematically and dynamically. In 1998 Collins [1] extended the factorization theorem to address the case of heavy quarks; this work provided the theoretical foundation that allows us to reliably compute heavy quark processes

[^109]throughout the full kinematic realm.

### 1.1. NLO DIS calculation

Figure 1 displays characteristic Feynman graphics for the first few orders of DIS heavy quark production. If we consider the DIS production of heavy quarks at $\mathcal{O}\left(\alpha_{S}^{1}\right)$ this involves the LO $Q V \rightarrow Q$ process and the NLO $g V \rightarrow Q \bar{Q}$ process.


Figure 1. Characteristic Feynman graphs which contribute to DIS heavy quark production: a) the LO $\mathcal{O}\left(\alpha_{S}^{0}\right)$ quark-boson scattering $Q V \rightarrow Q$, b) the NLO $\mathcal{O}\left(\alpha_{S}^{1}\right)$ gluon-boson scattering $g V \rightarrow$ $Q \bar{Q}$, and c) the NNLO $\mathcal{O}\left(\alpha_{S}^{2}\right)$ boson-gluon scattering $g V \rightarrow g Q \bar{Q}$.

The key ingredient provided by the ACOT scheme is the subtraction term (SUB) which removes the "double counting" arising from the regions of phase space where the LO and NLO contributions overlap. Specifically, the subtraction
term is:
$\sigma_{S U B}=f_{g} \otimes \tilde{P}_{g \rightarrow Q} \otimes \sigma_{Q V \rightarrow Q}$
$\sigma_{S U B}$ represents a gluon emitted from a proton $\left(f_{g}\right)$ which undergoes a collinear splitting to a heavy quark ( $\tilde{P}_{g \rightarrow Q}$ ) convoluted with the LO quark-boson scattering $\sigma_{Q V \rightarrow Q}$. Here, $\tilde{P}_{g \rightarrow Q}(x, \mu)=\frac{\alpha_{s}}{2 \pi} \ln \left(\mu^{2} / m_{c}^{2}\right) P_{g \rightarrow c}(x)$ where $P_{g \rightarrow c}(x)$ is the usual $\overline{M S}$ splitting kernel.

### 1.2. When do we need Heavy Quark PDFs

The novel ingredient in the above calculation is the inclusion of the heavy quark PDF contribution which resums logs of $\ln \left(\mu^{2} / m_{Q}^{2}\right)$. One can ask the question: When do we need to consider such terms? The answer is illustrated in Figure 2 where we compare the DGLAP evolved $\operatorname{PDF} f_{c}(x, \mu)$ with the single splitting perturbative result.

The DGLAP PDF evolution sums a nonperturbative infinite tower of logs while the SUB contribution removes the perturbative single splitting component which is already included in the NLO contribution. Hence, at the PDF level the difference between the heavy quark DGLAP evolved PDF $f_{Q}$ and the single-splitting perturbative $\tilde{f}_{Q}$ will indicate the contribution of the higher order logs which are resummed into the heavy quark PDF. Here, we shall find it convenient to define $\tilde{f}_{Q}=f_{g} \otimes \tilde{P}_{g \rightarrow Q}$ which represents the PDF of a heavy quark $Q$ generated from a single perturbative splitting.

For $\mu \sim m_{Q}$ we see that $f_{Q}$ and $\tilde{f}_{Q}$ match quite closely, whereas $f_{Q}$ and $\tilde{f}_{Q}$ differ significantly for $\mu$ values a few times $m_{Q}$. While the details will depend on the specific process, in general we find that for $\mu$ scales 3 to 5 times $m_{Q}$ the terms resummed by the heavy quark PDF can be significant.

## 2. The ACOT Renormalization Scheme

### 2.1. Massive vs. Massless Evolution

Another useful result that arises from the proof of Collins [1] is that we can use mass-independent (massless) evolution kernels to evolve the heavy quark PDFs without any loss of accuracy as compared to a mass-dependent (massive) evolution


Figure 2. Comparison of the DGLAP evolved charm $\operatorname{PDF} f_{c}(x, \mu)$ with the perturbatively computed single splitting (SUB) $f_{c}(x, \mu)=f_{g}(x, \mu) \otimes$ $\tilde{P}_{g \rightarrow c}$ charm evolution vs. $\mu$ in GeV for two representative values of $x$.
kernel. [ 2]. Specifically, Collins demonstrated that consistent application of the formalism correctly resums the massive contributions up to higher-twist corrections $\mathcal{O}\left(\Lambda_{Q C D}^{2} / Q^{2}\right)$ and that there are no errors of order $\mathcal{O}\left(m_{Q}^{2} / Q^{2}\right)$.
This result is illustrated in Figure 3 where we compare the results of a NLO DIS heavy quark production calculation using massless and massive DGLAP evolution kernels. In Fig. 3a) we see that while the choice of massive or massless kernels significantly changes the individual $L O$ and $S U B$ contributions, the difference $L O-S U B$ which contributes to the total ( $T O T=L O-$


Figure 3. Comparison of heavy quark DIS structure function for mass-dependent (massive) and massindependent (massless) evolution.
$S U B+N L O$ ) is minimal. This numerically verifies that the choice of massive or massless evolution kernels is purely a scheme choice which has no physical content.

While we see this result demonstrated numerically in Figure 3, the underlying reason for this result is closely related to the previous observations made regarding Figure 2. The LO result is given by $L O \sim f_{Q} \otimes \sigma_{Q \rightarrow Q}$ and the subtraction term is given by $S U B \sim f_{g} \otimes \tilde{P}_{g \rightarrow Q} \otimes \sigma_{Q \rightarrow Q}$. If we expand the DGLAP equation for $f_{Q}$ in the region $\mu \sim m_{Q}$ we find $f_{Q} \sim f_{g} \otimes \tilde{P}_{g \rightarrow Q}+\mathcal{O}\left(\alpha_{s}^{2}\right)$; thus, we have $L O \sim f_{g} \otimes \tilde{P}_{g \rightarrow Q} \otimes \sigma_{Q \rightarrow Q}+\mathcal{O}\left(\alpha_{S}^{2}\right)$. We observe that while $L O$ and $S U B$ individually depend on the specific splitting kernels, the combination $L O-S U B$ is insensitive to whether we use the massive or massless kernel. ${ }^{2}$

Therefore, we conclude that so long as the splitting kernels $P_{a \rightarrow b}$ are matched between the DGLAP evolution and the definition of the subtractions (SUB), the choice of a massive or massless DGLAP evolution kernel was purely a choice of scheme and the physical results are invariant.

### 2.2. S-ACOT

In a complementary application, it was observed that the heavy quark mass could be set to zero in certain pieces of the hard scattering terms without any loss of accuracy. This modi-

[^110]fication of the ACOT scheme goes by the name Simplified-ACOT (S-ACOT) and can be summarized as follows.

S-ACOT: For hard-scattering processes with incoming heavy quarks or with internal onshell cuts on a heavy quark line, the heavy quark mass can be set to zero ( $m_{Q}=0$ ) for these pieces [3].

If we consider the case of NLO DIS heavy quark production, this means we can set $m_{Q}=0$ for the LO terms ( $Q V \rightarrow Q$ ) as this involves an incoming heavy quark, and we can set $m_{Q}=0$ for the SUB terms as this has an on-shell cut on an internal heavy quark line. Hence, the only contribution which requires calculation with $m_{Q}$ retained is the NLO $g V \rightarrow Q \bar{Q}$ process.

Figure 4 displays a comparison of a calculation using the ACOT scheme with all masses retained vs. the S-ACOT scheme; as promised, these two results match throughout the full kinematic region.

### 2.3. ACOT- $\chi$

In the conventional implementation of the heavy quark PDFs, we must "rescale" the Bjorken $x$ variable as we have a massive parton in the final state. The original rescaling procedure is to make the substitution $x \rightarrow x\left(1+m_{c}^{2} / Q^{2}\right)$ which provides a kinematic penalty for producing the heavy charm quark in the final state [4]. As the charm is pair-produced by the $g \rightarrow c \bar{c}$ process, there are actually two charm quarks in the final


Figure 4. Comparison of schemes for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number (FFN), and Zero-Mass Variable Flavor Number (ZM-VFN) schemes. The ACOT and S-ACOT results are virtually identical.
state-one which is observed in the semi-leptonic decay, and one which goes down the beam pipe with the proton remnants. Thus, the appropriate rescaling is not $x \rightarrow x\left(1+m_{c}^{2} / Q^{2}\right)$ but instead $x \rightarrow \chi=x\left(1+\left(2 m_{c}\right)^{2} / Q^{2}\right)$; this rescaling is implemented in the ACOT- $\chi$ scheme, for example [ $5,6,7]$. The factor $\left(1+\left(2 m_{c}\right)^{2} / Q^{2}\right)$ represents a kinematic suppression factor which will suppress the charm process relative to the lighter quarks.

### 2.4. Numerical Comparison

Having introduced the various theoretical issues which enter the calculation of the heavy quark process, we illustrate the numerical size of these choices for the case of DIS heavy quark production.

In Figure 5 we display the charm structure function $F_{2}^{c}(x, \mu)$ for a variety of schemes and orders. LO represents the $\mathcal{O}\left(\alpha_{s}^{0}\right) Q V \rightarrow Q$ process. NLO includes the $\mathcal{O}\left(\alpha_{s}^{1}\right)$ processes (primarily $g V \rightarrow Q \bar{Q}$ ) in the massless approximation. In the Fixed-Flavor-Scheme (FFS) the heavy quark PDF is set to zero; hence, at $\mathcal{O}\left(\alpha_{s}^{1}\right)$ this only receives contributions from $g V \rightarrow Q \bar{Q}$. The ACOT and S-ACOT schemes are virtually identical-the curves are indistinguishable in this plot. Finally,


Figure 5. Calculation of DIS heavy quark production for a variety of schemes.
the implementation of the $\chi$-prescription for the S-ACOT scheme (the ACOT- $\chi$ would yield identical results) provides some additional suppression in the region $\mu \sim m_{Q}$. To this order, our best theoretical estimate of the true cross section would be either the ACOT- $\chi$ or equivalently S-ACOT- $\chi$.
To see the effect of these different results in the context of a global fit we display the results for the CTEQ6M and CTEQ6HQ PDFs sets in Table 1. Both the fits using a consistent application of the ACOT and $\overline{M S}$ schemes yield good results. In contrast, if we mismatch the scheme used in the PDF with that in the cross section calculation we observe a dramatic increase in the $\chi^{2}$ values obtained. This result underscores the importance of using properly matched calculations.

### 2.5. Heavy Quarks at the Tevatron

In the previous discussion we have primarily focused on DIS production of heavy quarks for illustrative purposes as the formalism is easier to layout when there is only a single hadron in the initial state. Nevertheless, the same principles that we have used in the the DIS case can be applied to that of the hadron-hadron initial state as appropriate for the Tevatron and the LHC.
Historically, the predictions of b-production at hadron-hadron colliders have been a challenge; the early results from the Tevatron were a factor of 2 to 3 larger than the theoretical predictions. NLO QCD corrections to the $\mathrm{LO} g g \rightarrow Q \bar{Q}$

| Set | \# points | CTEQ6HQ | CTEQ6M | 6M $\otimes$ GM | 6HQ $\otimes$ ZM |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ZEUS | 104 | 0.91 | 0.98 | 2.84 | 3.72 |
| H1 | 484 | 1.02 | 1.04 | 1.50 | 1.22 |
| TOTAL | 1925 | 1.04 | 1.06 | 1.26 | 1.30 |

Table 1
Table of $\chi^{2}$ per point for the individual HERA data sets, and for the TOTAL of all data sets. (Non-HERA data sets are not displayed.) The results are shown for CTEQ6HQ PDF using the General Mass (GM) ACOT scheme, and CTEQ6M PDF using the zero-mass (ZM) $\overline{M S}$ scheme. We note the increased $\chi^{2}$ for mixed schemes using CTEQ6M with the GM ACOT scheme, and the CTEQ6HQ with the ZM scheme.
process were formidable and yielded large corrections $[8,9,10,11,12]$. It is interesting to observe that if the heavy quark PDF is taken into account so that the LO contribution consists of both $g g \rightarrow Q \bar{Q}$ and $g Q \rightarrow g Q$, then the computed NLO contributions (with appropriate subtractions) are thereby reduced suggesting improved convergence of the perturbation theory $[13,14,15,16,17,18]$.

Ref. [ 19] performs a systematic comparison of the GM-VFNS and ZM-VFNS using results of an updated analysis of hadronic b-production at the Tevatron. Figure 6 displays these results for the Tevatron in the central rapidity region as compared with the CDF data [ 20,21 ]. The result is that the finite mass effects moderately enhance the $p_{T}$ distribution in the region $p_{T} \sim 2 m_{H}$ by about $20 \%$, and this enhancement decreases at larger $p_{T}$. For intermediate to large $p_{T}$ values ( $p_{T}>m_{H}$ ) the three calculations (GM-VFNS, ZM-VFNS, FFN) match quite closely, and are in good agreement with the data. Conversely, if we use the FFN result with the historic values for the PDF and $\alpha_{S}$ we find this prediction is roughly a factor of 3 below the data.

The excellent agreement between data and theory for this process is an important achievement and represents the culmination of many years of effort by both the theoretical and experimental community.

## 3. Schemes used for Global Analysis

The ACOT scheme and variants were used for the CTEQ series of global PDF fits. ${ }^{3}$ For the MRST/MSTW series of global PDF fits the

[^111]

Figure 6. From Ref. [ 19], the transverse momentum distribution $d \sigma / d p_{T}$ for $p \bar{p} \rightarrow B X$ at $\sqrt{s}=1.96 \mathrm{TeV}$. The results are shown for the General Mass (GM) Variable Flavor Number (VFN) scheme and the Zero Mass (ZM) Variable Flavor Number (VFN) scheme. Additionally, results are shown for the Fixed Flavor Number (FFN) scheme with both recent PDFs (dot-dashed line) and the historical PDFs (dotted line). The data is from the CDF collaboration [ 20, 21].


Figure 7. Diagrammatic comparison of TR and ACOT type schemes for the case of DIS. This diagram is schematic to emphasize the similarities and differences. The leading-order (LO) process is a $\mathcal{O}\left(\alpha_{s}^{0}\right)$ boson scattering from a heavy quark, e.g. $\gamma Q \rightarrow Q$; the NLO $\mathcal{O}\left(\alpha_{S}^{1}\right)$ correction arises from $\gamma g \rightarrow Q \bar{Q}$, and the NNLO $\mathcal{O}\left(\alpha_{S}^{2}\right)$ correction arises from $\gamma g \rightarrow Q \bar{Q} g$.

Thorne-Roberts (TR) scheme was used. As these two sets of PDFs are widely used it is of interest to compare and contrast these approaches. Figure 7 displays a diagrammatic comparison of the TR [ 22, 23] and ACOT type schemes. While these schemes may appear quite different at first glance, they differ by higher-order terms which will be reduced as we increase the order of our perturbation theory.

In perturbation theory, we compute our observables to a fixed order $N$ in $\alpha_{S}$; hence, we truncate the perturbation expansion at $\mathcal{O}\left(\alpha_{S}^{N}\right)$, and we have neglected terms of order $\mathcal{O}\left(\alpha_{S}^{N+1}\right)$. In brief, the difference between these two approaches amounts to adding different $\mathcal{O}\left(\alpha_{S}^{N+1}\right)$ higher order terms. Thus, these two approaches will agree on the contributions up to $\mathcal{O}\left(\alpha_{S}^{N}\right)$. We will now review the motivation and consequences of adding the differing higher order terms.

### 3.1. Leading-Order (LO) $\left(\alpha_{S}^{0}\right)$

If we work at Leading-Order ${ }^{4}$ (LO) $\alpha_{S}^{0}$, when the heavy quark PDF is an "active" parton (typically $\mu>m_{H}$ ) the LO contribution is $\gamma+Q \rightarrow Q$. However, when the heavy quark PDF is not an "active" parton (typically $\mu<m_{H}$ ) the LO contribution vanishes. For the ACOT scheme, no higher order terms are added to this results. Hence for scales $\mu<m_{H}$, the LO answer is zero and we expect large corrections to this result at NLO. For the TR scheme, a portion of the $\gamma g \rightarrow Q \bar{Q}$ contribution is added; for $\mu<m_{H}$ the full $\gamma g \rightarrow Q \bar{Q}$ term is included, and for $\mu>m_{H}$ the $\gamma g \rightarrow Q \bar{Q}$ term frozen at $\mu=Q=m_{H}$ to avoid any difficulty with large logarithms of the form $\ln \left(m_{H} / \mu\right)$.

Consequently, in the $\mu<m_{H}$ region the TR

[^112]scheme yields a finite LO result while the ACOT scheme yields zero. While both schemes formally agree at $\mathcal{O}\left(\alpha_{S}^{0}\right)$, clearly the $\mathcal{O}\left(\alpha_{S}^{1}\right)$ terms can be important, particularly in the $\mu<m_{H}$ region.

### 3.2. Next-to-Leading-Order (NLO) $\left(\alpha_{S}^{1}\right)$

If we work at $\mathrm{NLO}\left(\alpha_{S}^{1}\right)$, for the low $\mu$ region we now include $\gamma g \rightarrow Q \bar{Q}$ as well as the $\gamma+Q \rightarrow Q$ process. ${ }^{5}$ If we again look in the region $\mu<m_{H}$, we find that while the ACOT scheme yielded zero at LO, it now obtains a finite result at NLO. For the TR scheme, in addition to the above terms, a portion of the $\gamma g \rightarrow g Q \bar{Q}$ contribution is added; again, for $\mu>m_{H}$ the $\gamma g \rightarrow g Q \bar{Q}$ term is frozen at $\mu=Q=m_{H}$ to avoid any difficulty with large logarithms.

As before, both the TR scheme and ACOT scheme formally agree at $\mathcal{O}\left(\alpha_{S}^{1}\right)$, but they will differ by the separate NNLO $\mathcal{O}\left(\alpha_{S}^{2}\right)$ terms that have been included. In contrast to the LO case where the ACOT scheme yielded zero for $\mu<m_{H}$, both schemes give finite results in all kinematic regions; hence, the relative difference will be reduced.

### 3.3. General Comparisons at Order $\alpha_{S}^{N}$

Let us make some observations regarding these schemes at a general order in perturbation $\mathcal{O}\left(\alpha_{S}^{N}\right)$. We observe that for a given set of processes calculated to $\alpha_{s}^{N}$, we can implement the TR scheme to $\mathcal{O}\left(\alpha_{S}^{N-1}\right)$ and the ACOT scheme to $\mathcal{O}\left(\alpha_{S}^{N}\right)$. For example, at NLO we note that the ACOT scheme involves only graphs of order $\alpha_{s}^{1}$ while TR utilizes graphs of order $\alpha_{s}^{2}$. At present we know the $\mathcal{O}\left(\alpha_{S}^{2}\right)$ massive neutral current process $(\gamma g \rightarrow g Q \bar{Q} ; \gamma Q \rightarrow g g Q$ and associated graphs); hence, this allows us to compute the TR scheme to $\mathcal{O}\left(\alpha_{S}^{1}\right)$ and the ACOT scheme to $\mathcal{O}\left(\alpha_{S}^{2}\right)$. In contrast, the massive charged current process is known only to $\mathcal{O}\left(\alpha_{S}^{1}\right)$; hence, this allows us to compute the TR scheme to $\mathcal{O}\left(\alpha_{S}^{0}\right)$ and the ACOT scheme to $\mathcal{O}\left(\alpha_{S}^{1}\right)$.

We note that recent improvements of theoretical techniques have enabled significant advances in the calculation higher-order heavy quark pro-

[^113]cesses. For example, Ref. [ 25] has obtained the asymptotic results for $F_{L}^{Q \bar{Q}}(x, \mu)$ at the 3-loop order, and recently Ref. [ 26] has extended this work for the case of $F_{2}^{Q \bar{Q}}(x, \mu)$.

In general, the TR scheme achieves in practice the same highest asymptotic order as ACOT by some modeling of terms below $Q^{2}=m_{Q}^{2}$ which become (relatively) unimportant at high $Q^{2}$. As we move to higher order calculations, the differences between these schemes will be reduced as they arise from uncalculated higher-order contributions.

## 4. NNLO and Beyond

Although NLO is the state-of-the-art for many calculations, improved experimental precision demands that we strive toward a NNLO accuracy. When we consider PDFs for heavy quarks at NNLO, there are a number of new elements that enter.

One consequence is that the PDFs are no longer continuous across the heavy flavor threshold. Even more, when matching charm and bottom across their thresholds, they start from negative values as illustrated in Figure 8. The matching conditions have been computed by a number of groups [ 27, 28], and at NNLO PDFs will have


Figure 8. The b-quark PDF $x f_{b}(x, Q)$ with NNLO matching conditions for 3 choices of $x$.
discontinuities of order $\mathcal{O}\left(\alpha_{S}^{2}\right)$ when we transition from $N_{F}$ to $N_{F}+1$ flavors. While we may be uncomfortable with discontinuities in our PDFs, we are reminded that the PDFs are not physical observables, but instead are only theoretical constructs which depend on (arbitrary) renormalization schemes and scales. ${ }^{6}$

At NLO, the point $\mu=m_{Q}$ is special because $f_{a}^{N_{F}}\left(x, m_{Q}\right)=f_{a}^{N_{F}+1}\left(x, m_{Q}\right)$; this is because the constant term in the matching equation happens to be zero at NLO. Because of this "accident" it was common to use $\mu=m_{Q}$ as both the Matching Point and the Transition Point.

At NNLO the point $\mu=m_{Q}$ no longer has these special properties as the transition from $N_{F}$ to $N_{F}+1$ will necessarily have discontinuities at any value of $\mu$; hence, it may be desirable to choose the Matching Point and the Transition Point at different values of $\mu$. As these two point are not usually distinguished, let us highlight their key features.

Matching Point $\mu_{M}$ : The value of $\mu$ where the $N_{F}+1$ scheme is defined in terms of the $N_{F}$ scheme by a relation of the form: $f_{a}^{N_{F}+1}(x, \mu)=A_{a b} \otimes f_{b}^{N_{F}}(x, \mu)$.
Transition Point $\mu_{T}$ : The value of $\mu$ where the user chooses to transition from the $N_{F}$ scheme to the $N_{F}+1$ scheme.

Figure 9 schematically represents how each calculation with a set number of flavors $N_{F}$ has a particular region of applicability where it is best suited to describe the "true" physics. The complete description of the physics throughout the full kinematic range will therefore consist of a patchwork of schemes which are "sewn together."

The Transition Point: It is easy to imagine situations where we would not want to automatically transition between schemes at $\mu=m_{Q}$. For example, consider we are analyzing data in the range $\mu \in[2,5] \mathrm{GeV}$. The bulk of the range is in the $N_{F}=4$ flavor region as $\mu>m_{c} \sim 1.3 \mathrm{GeV}$,

[^114]

Figure 9. The upper figure schematically represents how each calculation with a set number of flavors $N_{F}$ has a region of applicability. The transition from the $N_{F}-1$ scheme to the $N_{F}$ scheme should be in the vicinity of the $m_{N_{F}}$ mass, but need not occur exactly at $\mu=m_{N_{F}}$. The lower figure illustrates that multiple PDFs can coexist for $\mu \geq m_{N_{F}}$ with matching performed at $\mu=m_{N_{F}}$.
but a small portion of the range extends above the $N_{F}=5$ flavor region as $\mu>m_{b} \sim 4.5 \mathrm{GeV}$. In the region $\mu \in[4.5,5] \mathrm{GeV}$ it would be inconvenient to be forced to transition to a $N_{F}=5$ scheme because 1) the b-quark clearly plays no substantive role in this kinematic range, and 2) both the PDFs and $\alpha_{s}(\mu)$ will have discontinuities at $\mu=m_{b}$.

Clearly it is more reasonable to have the option to work consistently in a $N_{F}=4$ flavor scheme even for $\mu \gtrsim m_{b}$. If PDFs were generated such that the $N_{F}=4$ and $N_{F}=5$ schemes co-exist in the region $\mu \sim m_{b}$, then the user could select $N_{F}$ by choice.
The lower portion of Figure 9 illustrates how this might be implemented. The PDFs can be generated such that the $N_{F}$ scheme is available for all $\mu \geq m_{N_{F}}$. Thus, for $\mu=5 \mathrm{GeV}$ the user
would have access to schemes with $N_{F}=\{3,4,5\}$ and can select the scheme by specifying $N_{F}$ in addition to $\{x, \mu\}$. Therefore, the user could analyze their $\mu \in[2,5] \mathrm{GeV}$ data set consistently in a single $N_{F}=4$ scheme, and choose to transition to the $N_{F}=5$ scheme at a higher $\mu$ value to be specified by the user.

The Matching Point: Although the Matching Point can be set to any $\mu$ value in the region of $m_{N_{F}}$, we shall argue that the choice $\mu_{M}=m_{N_{F}}$ is optimal.

First, we note that the Matching Point should be at or below the Transition Point $\left(\mu_{T} \geq \mu_{M}\right)$ if we desire to avoid downward DGLAP evolution (which can be unstable). Therefore, if we perform the matching at the heavy quark mass we have the reasonable constraint: $\mu_{T} \geq \mu_{M}=m_{N_{F}}$.

Second, the matching conditions which define $f_{a}^{N_{F}+1}$ in terms of $f_{a}^{N_{F}}$ are of the form $f_{a}^{N_{F}+1}=$ $A_{a b} \otimes f_{b}^{N_{F}}$ with
$A_{a b}=\delta_{a b}+\frac{\alpha_{s}}{2 \pi} P_{b \rightarrow a}\left[\ln \left(\frac{\mu^{2}}{m_{Q}^{2}}\right)+c_{b \rightarrow a}\right]$
up to $O\left(\alpha_{s}^{2}\right)$. Here, $P_{b \rightarrow a}$ is the DGLAP splitting kernel and $c_{b \rightarrow a}$ is a constant. ${ }^{7}$ The choice $\mu_{M}=m_{N_{F}}$ eliminates the logarithmic terms thus simplifying the calculation.

We also observe that shifting the Matching Point from $m_{Q}$ to $2 m_{Q}$ does not suppress the heavy quark PDF as the logarithmic terms compensate for evolution between $m_{Q}$ and $2 m_{Q}$.

## 5. Conclusions:

The computation of heavy quark production has historically been challenging both theoretically and experimentally. On the theoretical side, the heavy quark introduces an additional mass scale which complicates the calculations. On the experimental side, the data for heavy quark production has typically differed from the theoretical

[^115]predictions by a significant factor. Recent theoretical developments enable us to incorporate the heavy quark mass into the calculation both dynamically and kinematically. These calculations have been used to produce matched PDFs incorporating the full mass dependence. Updated analyses show improved agreement between data and theory for both HERA and Tevatron measurements.
Improved experimental precision will demand NNLO accuracy from the theoretical calculations, and this introduces a number of issues not present at the NLO order. There is progress underway on both the PDFs and the hard-scattering calculations, and this should ensure we are well prepared for the upcoming LHC data.
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# THE SM AND NLO MULTILEG AND SM MC WORKING GROUPS: Summary Report 

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#### Abstract

The 2011 Les Houches workshop was the first to confront LHC data. In the two years since the previous workshop there have been significant advances in both soft and hard QCD, particularly in the areas of multi-leg NLO calculations, the inclusion of those NLO calculations into parton shower Monte Carlos, and the tuning of the non-perturbative parameters of those Monte Carlos. These proceedings describe the theoretical advances that have taken place, the impact of the early LHC data, and the areas for future development.


Report of the SM and NLO Multileg and SM MC Working Groups for the Workshop "Physics at TeV Colliders", Les Houches, France, 31 May-8 June, 2011.

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## Part I

## INTRODUCTION

The workshop in 2011 was the first for which the long-awaited LHC data (at 7 TeV ) was available for analysis and comparison to theory. Even though of limited statistical power compared to the ultimate goals of the LHC, this data accesses a very wide kinematic range, and probes regions where multiple scales are important. The presence of large scales for some processes, on the TeV level, points to the importance of electroweak corrections, which have been calculated only for some of the important processes. The first hints of a Higgs boson have now been observed. In order to search for signs of New Physics, as well as to completely understand the Standard Model at the LHC, it is important to understand the perturbative framework at the LHC. The data taken so far provides many challenges for perturbative QCD predictions; and it is clear that New Physics, if it is present in current data, is hiding well.

On the theoretical side, there has been a great deal of productivity in the area of multi-particle calculations at next-to-leading order (NLO) and next-to-next-to-leading order (NNLO). NLO is the first order at which the normalization, and in some cases the shape, of perturbative cross sections can be considered reliable [1]. A full understanding for both Standard Model and beyond the Standard Model physics at the LHC requires the development of fast, reliable programs for the calculation of multi-parton final states at NLO. There have been many advances in the development of NLO techniques, especially in the area of automation $[2,3,4,5,6,7,8,9,10,11,12]$.

Some of these approaches also allow for relatively easy [13, 14, 12] and/or automatic [15] inclusion of the NLO matrix elements into parton shower Monte Carlo programs. For more details we refer to the individual contributions in these proceedings.

A prioritized list of NLO (and some NNLO) cross sections was assembled at Les Houches in 2005 [16] and added to in 2007 [17] and 2009 [18]. This list includes cross sections which are experimentally important, and which are theoretically feasible (if difficult) to calculate. As we stand now, basically all NLO $2 \rightarrow 3$ and $2 \rightarrow 4$ cross sections of interest have been calculated, see Tables 12 below, and even some processes which were not on the 2009 wishlist are available at NLO, see e.g. [19, 20, 21, 22, 23, 24, 25]. The success of automation techniques means that future NLO calculations of similar complexity can be completed without the man-years of labor previously required. Thus, we do not add to the NLO wish list in 2011. Instead, we comment on calculations needed at NNLO, and processes at NLO for which it is important to calculate the impact of electroweak corrections, and/or the
influence of interference effects with other processes with the same final state.
For many of the processes calculated at the LHC (such as for Higgs production), it is important either to apply a veto for the production of extra jets, or to bin the analysis results according to the jet multiplicity. While such cuts are useful for dealing with the experimental backgrounds, the exclusivity of the cross sections results in increases to the theoretical uncertainties obtained for the corresponding inclusive results, see e.g. [26]. The impact of such cuts is explored in the contribution of Stewart and Tackmann in these proceedings.

Much of the complexity for multi-parton NLO processes consists of the calculation of the nonleading color contributions. Such contributions typically contribute only at the level of a few percent and approximations to the non-leading color contributions should be accurate within a percent or so [70, 71, [51]. So it may be more time-prudent for groups carrying out such calculations to estimate the non-leading color effects before carrying out the full calculation.

To reach full utility, the codes for any of these complex NLO calculations should be made public and/or the authors should generate ROOT ntuples providing the parton level event information from which experimentalists can assemble any cross sections of interest. Where possible, decays (with spin correlations) should be included. A ROOT output option is especially useful where the creation of a user-friendly NLO program may be very time-consuming. We now have some experience with the use of ROOT ntuples with both MCFM and Blackhat+Sherpa calculations. The latter, in particular, does not exist as a public program, while ROOT tuples have been made available for NLO W/Z +n jet multiplicities (with $n$ up to 4 ) for $W / Z+$ jets, and (also for $n$ up to 4 ) for inclusive jet production. The estimation of the correct scale for use in multi-parton NLO calculations, and the proper evaluation of the uncertainty on this scale, is more complex than for simpler calculations. The use of ROOT ntuples can make these evaluations easier to carry out. A contribution describing their use has been included in these proceedings.

While NLO is sufficient for most predictions, it is also crucial to understand certain critical cross sections at NNLO. To date, NNLO calculations have been carried out primarily for processes in $e^{+} e^{-}$ annihilation [72, 73, 74], and in hadronic collisions for $2 \rightarrow 1$ processes, with the exception of VH [75, 76, 77] and $\gamma \gamma$ production [78].

To calculate a $2 \rightarrow 2$ scattering process at NNLO, the divergent contributions arising from the treelevel $2 \rightarrow 4$, the one-loop $2 \rightarrow 3$ and the two-loop $2 \rightarrow 2$ subprocesses have to be properly subtracted and cancelled, such that the finite remainders can be combined into a parton-level event generator. To combine the three contributions, an infra-red subtraction scheme for unresolved real radiation is required. Several approaches have been used and are being further developed: antenna subtraction [79], which currently is extended to hadronic and semi-hadronic initial states [80, 81, 82, 83, 84], a method based on sector decomposition appplied to real radiation [85, 86, 87] where the decomposition is guided by the physical singularity structure [88, 89], $q_{T}$-subtraction [90], which is very elegant but appplicable only to colourless final states, and the one of [91] described in these proceedings.

Further, two-loop amplitudes are interesting in their own right from a field theory point of view, for example to study asymptotic behaviour, or to gain insights into the all-order infared structure of massless field theories.

Below we construct a table of calculations needed at the LHC, and which are feasible within the next few years. Certainly, results for inclusive cross sections at NNLO will be easier to achieve than differential distributions, but most groups are working towards a partonic Monte Carlo program capable of producing fully differential distributions for measured observables.

- $t \bar{t}$ production:
needed for accurate background estimates, top mass measurement, top quark asymmetry (which is zero at tree level, so NLO is the leading non-vanishing order for this observable, and a discrepancy of theory predictions with Tevatron data needs to be understood). Several groups are already well


Table 1: The updated experimenter's wishlist for LHC processes

| Calculations beyond NLO added in 2007 |  |
| :--- | :--- |
| 13. $g g \rightarrow W^{*} W^{*} \mathcal{O}\left(\alpha^{2} \alpha_{s}^{3}\right)$ | backgrounds to Higgs |
| normalization of a benchmark process |  |
| 14. NNLO $p p \rightarrow t \bar{t}$ |  |
| 15. NNLO to VBF and $Z / \gamma+$ jet |  |
| Calculations including electroweak effects |  |
| 16. NNLO QCD+NLO EW for $W / Z$ | precision calculation of a SM benchmark |
| NLO EW to $W / Z$ | $[65,66$ |
| NLO EW to $W / Z+$ jet |  |
| NLO EW to $W H / Z H$ | $[67,6]$ |
| $[69]$ |  |

Table 2: The updated experimenter's wishlist for LHC processes continued
on the way to complete NNLO results for $t \bar{t}$ production [92, 93, 94, 95].

- $W^{+} W^{-}$production:
importand background to Higgs search. At the LHC, $g g \rightarrow W W$ is the dominant subprocess, but $g g \rightarrow W W$ is a loop-induced process, such that two loops need to be calculated to get a reliable estimate of the cross section. Advances towards the full two-loop result are reported in [96, 97].
- inclusive jet/dijet production:

NNLO parton distribution function (PDF) fits are starting to become the norm for predictions and comparisons at the LHC. Paramount in these global fits is the use of inclusive jet production to tie down the behavior of the gluon distribution, especially at high $x$. However, while the other essential processes used in the global fitting are known to NNLO, the inclusive jet production cross section is only known at NLO. Thus, it is crucial for precision predictions for the LHC for the NNLO corrections for this process to be calculated, and to be available for inclusion in the global PDF fits. First results for the real-virtual and double real corrections to gluon scattering can be found in [98, 99].

- $\mathrm{V}+1$ jet production:
$W / Z / \gamma+$ jet production form the signal channels (and backgrounds) for many key physics processes, for both SM and BSM. In addition, they also serve as calibration tools for the jet energy scale and for the crucial understanding of the missing transverse energy resolution. The two-loop amplitudes for this process are known [100, 101], therefore it can be calculated once the parts involving unresolved real radiation are available.
- $\mathrm{V}+\gamma$ production:
important signal/background processes for Higgs and New Physics searches. The two-loop helicity amplitudes for $q \bar{q} \rightarrow W^{ \pm} \gamma$ and $q \bar{q} \rightarrow Z^{0} \gamma$ recently have become available [102].
- Higgs+1 jet production:

As mentioned previously, events in many of the experimental Higgs analyses are separated by the number of additional jets accompanying the Higgs boson. In many searches, the Higgs +0 jet and Higgs +1 jet bins contribute approximately equally to the sensitivity. It is thus necessary to have the same theoretical accuracy for the Higgs +1 jet cross section as already exists for the inclusive Higgs cross section, i.e. NNLO. The two-Loop QCD Corrections to the Helicity Amplitudes for $H \rightarrow 3$ partons are already available [103].

The contributions in this document are arranged as follows. In section II various developments concerning techniques for NLO and NNLO calculations are described, in particular in view of providing
automated tools for NLO corrections. In section III, issues related to parton distribution functions are discussed. Section IV contains phenomenological studies of observables and uncertainties, based on theory input where higher order corrections obtained by different approaches are available. Section V includes phenomenological studies on the definition of experimental observables and corrections applied to data. Finally Section VI discusses issues related to the tuning of Monte Carlos and standardised Monte Carlo output formats.

## Part II

## NLO AUTOMATION AND (N)NLO TECHNIQUES

## 1. PJFRY - A C++ PACKAGE FOR TENSOR REDUCTION OF ONE-LOOP FEYNMAN INTEGRALS ${ }^{1}$


#### Abstract

The C++ package PJFry 1.0.0 [104, 105] - a one loop tensor integral library is introduced. We use an algebraic approach to tensor reduction. As a result, the tensor integrals are presented in terms of scalar one- to four-point functions, which have to be provided by an external library, e.g. QCDLoop/FF or OneLOop or LoopTools/FF. The reduction is implemented until five-point functions of rank five. A numerical example is shown, including a special treatment for small or vanishing inverse four-point Gram determinants. Future modules of PJFry might cover the treatment of $n$-point functions with $n \geq 6$; the corresponding formulae are worked out. Further, an extremely efficient approach to tensor reduction relies on evaluations of complete contractions of the tensor integrals with external momenta. For this, we worked out an algorithm for the analytical evaluation of sums over products of signed minors with scalar products of chords, i.e. differences of external momenta. As a result, the usual multiple sums over tensor coefficients are replaced for the numerical evaluation by compact combinations of the basic scalar functions.


### 1.1 PJFry

The goal of the C++ package PJFry is a stable and fast open-source implementation of one-loop tensor reduction of Feynman integrals

$$
\begin{equation*}
I_{n}^{\mu_{1} \cdots \mu_{R}}=C(\epsilon) \int \frac{d^{d} k}{i \pi^{d / 2}} \frac{\prod_{r=1}^{R} k^{\mu_{r}}}{\prod_{j=1}^{n}\left(k-q_{j}\right)^{2}-m_{j}^{2}+i \epsilon}, \tag{1}
\end{equation*}
$$

suitable for any physically relevant kinematics ${ }^{2}$ The algorithm was invented in [105]. PJFry performs the reduction of 5 -point 1 -loop tensor integrals up to rank 5 . The 4 - and 3 -point tensor integrals are obtained as a by-product. Main features are:

- Any combination of internal or external masses
- Automatic selection of optimal formula for each coefficient
- Leading ()$_{5}$ are eliminated in the reduction

[^116]- Small ()$_{4}$ are avoided using asymptotic expansions where appropriate
- Cache system for tensor coefficients and signed minors
- Interfaces for C, C++, FORTRAN and Mathematica
- Uses QCDLoop [109, 110] or OneLOop [111] for 4-dim scalar integrals
- Available from the project webpage https://github.com/Vayu/PJFry/ [104, 105]

The installation of PJFry may be performed following the instructions given at the project webpage. The project subdirectories are ./src - the library source code ./mlink - the MathLink interface
./examples - the FORTRAN examples of library use, built with make check
A build on Unix/Linux and similar systems is done in a standard way by sequential performing ./configure, make, make install. See the INSTALL file for a detailed description of the ./configure options.

The functions for tensor coefficients for up to rank $R=5$ pentagon integrals are declared in the Mathematica interface:

```
In:= Names["PJFry`*"]
Out={A0v0, B0v0, B0v1, B0v2, C0v0, C0v1, C0v2, C0v3, \
D0v0, D0v1, D0v2, D0v3, D0v4, E0v0, E0v1, E0v2, \
EOv3, EOv4, EOv5, GetMu2, SetMu2}
```

The C++ and Fortran interface syntax is very close to that of e.g. LoopTools/FF:
E0v3[i,j,k,p1s,p2s,p3s,p4s,p5s,s12,s23,s34,s45,s15,m1s,m2s,m3s,m4s,m5s,ep=0]
where 3
i, $\mathrm{j}, \mathrm{k}$ are indices of the tensor coefficient $(0<i \leq j \leq k<n)$,
$\mathrm{p} 1 \mathrm{~s}, \mathrm{p} 2 \mathrm{~s}, \ldots$ are squared external masses $p_{i}^{2}$,
s12, s23, ... are Mandelstam invariants $\left(p_{i}+p_{j}\right)^{2}$,
$\mathrm{m} 1 \mathrm{~s}, \mathrm{~m} 2 \mathrm{~s}, \ldots$ are squared internal masses $m_{i}^{2}$,
$\mathrm{ep}=0,-1,-2$ selects the coefficient of the $\epsilon$-expansion.
The average evaluation time per phase-space point on a 2 GHz Core 2 laptop for the evaluation of all 81 rank 5 tensor form-factors amounts to 2 ms .

A numerical example is shown, for a configuration as in figure 1, in figures 2 and 3 for a five-point rank $R=4$ tensor coefficient in a region, where one of the 4-point sub-Gram determinants vanishes [at $x=0]$ :
$E_{3333}\left(0,0,-6 \times 10^{4}(x+1), 0,0,10^{4},-3.5 \times 10^{4}, 2 \times 10^{4},-4 \times 10^{4}, 1.5 \times 10^{4}, 0,6550,0,0,8315\right)$
The red curve is produced with standard PJFry, and the blue one with Passarino-Veltman [PV] reduction [112]; we mention that for the case treated here $(x \rightarrow 0)$, the PV reduction is no standard option. Our expansion in terms of higher dimensional scalar 3-point functions in case of vanishing 4-point subGram determinants uses only functions $I_{3}^{d+2 l}$ [105]. These are tensor coefficients of the pure $g^{\mu \nu}$ type [113], and so our method is different from others with a mixed numerical approach [114] or with use of additional tensor coefficients [115].

Tensor reduction by PJFry is used as one option of the GoSam package [12]. An older version of the algorithm, as described in [116], has been implemented independently in [11].

[^117]

Fig. 1: Momenta definitions for PJFry.

### 1.2 POTENTIAL UPGRADES

### 1.21 Tensor reduction for higher-point functions

So far, PJFry is foreseen for 5-point functions and simpler ones. The extension to 6-point functions is known from e.g. [114, 115, [116]. In [107] we solve analytically generalized recursions for $n \geq 6$, derived in [114]:

$$
\begin{equation*}
I_{n}^{\mu_{1} \mu_{2} \ldots \mu_{R}}=-\sum_{r=1}^{n} C_{r}^{\mu_{1}}(n) I_{n-1}^{\mu_{2} \cdots \mu_{R}, r} \tag{2}
\end{equation*}
$$

where in $I_{n-1}^{\mu, \cdots, r}$ the line $r$ is scratched. The coefficients for 6-point functions are:

$$
\begin{equation*}
C_{r}^{s, \mu}(6)=\sum_{i=1}^{5} \frac{1}{\binom{0}{s}_{6}}\binom{0 r}{s i}_{6} q_{i}^{\mu_{1}}, s=0 \ldots 6, \tag{3}
\end{equation*}
$$

where the $q_{i}$ are chords, and $\binom{0 r}{s i}_{6}$ etc. are signed minors with arbitrary $s$. For the 7-point and 8-point functions, we found several representations, among them

$$
\begin{equation*}
C_{r}^{s t, \mu}(7)=\sum_{i=1}^{6} \frac{1}{\binom{(t)^{2}}{s t}_{7}}\binom{s t i}{s t r}_{7} q_{i}^{\mu} \tag{4}
\end{equation*}
$$

and

$$
\begin{equation*}
C_{r}^{s t u, \mu}(8)=\sum_{i=1}^{7} \frac{1}{\binom{s t u}{s t u}_{8}}\binom{\text { stui }}{\text { stur }}_{8} q_{i}^{\mu} \tag{5}
\end{equation*}
$$

The upper indices $s, t$ and $u$ stand for the redundancy of the solutions and can be freely chosen.

### 1.22 Evaluation of contracted tensor integrals using sums over signed minors

The contraction of a tensor integral with chords may be written as a sum over basic scalar integrals (at a stage where they are free of tensor coefficient indices), multiplied by (multiple) sums over chords times


Fig. 2: Absolute accuracy of $E_{3333}$ in the region of vanishing sub-Gram determinant. Blue curve: conventional Passarino-Veltman reduction, red curve: PJFry.
signed minors. If one may perform these sums algebraically, the method becomes very efficient. And this has been systematically worked out in [106], see also [108].

We reproduce here two 7-point examples.
The rank $R=2,3$ integrals become by contraction

$$
\begin{align*}
q_{a, \mu} q_{b, \nu} I_{7}^{\mu \nu} & =\sum_{r, t=1}^{7} K^{a b, r t} I_{5}^{r t},  \tag{6}\\
q_{a, \mu} q_{b, \nu} q_{c, \lambda} I_{7}^{\mu \nu \lambda} & =\sum_{r, t, u=1}^{7} K^{a b c, r t u} I_{4}^{r t u}, \tag{7}
\end{align*}
$$

where $I_{5}^{r t}$ and $I_{4}^{r t u}$ are scalar 5- and 4-point functions, arising from the 7-point function by scratching lines $r, t, \ldots$ In the general case, we have at this stage higher-dimensional integrals $I_{n}^{d+2 l}, n=2, \ldots, 5$, to be further reduced following the known scheme, if needed. Here, the $I_{5}^{r t}$ have to be expressed by 4 -point functions.

The expansion coefficients are factorizing here,

$$
\begin{align*}
K^{a b, r t} & =K^{a, r} K^{b, r t},  \tag{8}\\
K^{a b c, r t u} & =-K^{a, r} K^{b, r t} K^{c, r t u} \tag{9}
\end{align*}
$$

and the sums over signed minors have been performed analytically:

$$
\begin{gather*}
K^{a, r}=\frac{1}{2}\left(\delta_{a r}-\delta_{7 r}\right),  \tag{10}\\
K^{b, r t}=\sum_{j=1}^{6}\left(q_{b} q_{j}\right) \frac{\left(\begin{array}{c}
r s t \\
r s)_{7}
\end{array}\right.}{\binom{r s}{r s}_{7}} \equiv \frac{\Sigma_{b}^{1, s t u}}{\binom{r s}{r s}_{7}}=\frac{1}{2}\left(\delta_{b t}-\delta_{7 t}\right)-\frac{1}{2} \frac{\binom{r s}{t s}_{7}}{\binom{r s}{r s}}\left(\delta_{b r}-\delta_{7 r}\right), \tag{11}
\end{gather*}
$$



Fig. 3: Relative accuracy of $E_{3333}$ in the region of vanishing sub-Gram determinant. At $x \sim 0.0015$, PJFry switched to the asymptotic expansion.

$$
\begin{align*}
K^{a, s t u} & =\sum_{i=1}^{6}\left(q_{a} q_{i}\right)\binom{0 s t u}{0 s t i}_{7} \equiv \Sigma_{a}^{2, s t u}  \tag{12}\\
& =\frac{1}{2}\left\{\binom{s t u}{s t 0}_{7}\left(Y_{a 7}-Y_{77}\right)+\binom{0 s t}{0 s t}_{7}\left(\delta_{a u}-\delta_{7 u}\right)-\binom{0 s t}{0 s u}_{7}\left(\delta_{a t}-\delta_{7 t}\right)-\binom{0 t s}{0 t u}_{7}\left(\delta_{a s}-\delta_{7 s}\right)\right\}
\end{align*}
$$

with

$$
\begin{equation*}
Y_{j k}=-\left(q_{j}-q_{k}\right)^{2}+m_{j}^{2}+m_{k}^{2} \tag{13}
\end{equation*}
$$

Conventionally, $q_{7}=0$.
The sums may be found in eqns. (A.15) and (A.16) of [106]. The $s$ is redundant and fulfils $s \neq r, b, 7$ in $K^{b, r t}$. In $K_{0}^{a, s t u}$ it is $s, t, u=1, \ldots 7$ with $s \neq u, t \neq u$.

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## 2. THE GOSAM APPROACH TO AUTOMATED ONE-LOOP CALCULATIONS ${ }^{4}$


#### Abstract

We describe the GoSAM framework for the automated computation of multiparticle scattering amplitudes at the one-loop level. The amplitudes are generated explicitly in terms of Feynman diagrams, and can be evaluated using either $d$-dimensional reduction at the integrand level or tensor decomposition. GoSAM can be used to compute one-loop QCD and EW corrections to Standard Model processes, and it is ready to link generic model files for theories Beyond the Standard Model.


[^118]
### 2.1 Introduction and General Motivations

In the last few years we observed major advances in the direction of constructing packages for fully automated one-loop calculations, which profited from the new developments in the field of NLO QCD calculations [17, 18]. The continuous improvement of the techniques for one-loop computations led to important new results for processes with many particles [51, 70, 117, 71, 53, 48, 49, 50, 54, 62, 63, 23, 118, 25, 56, 57, 21, 22, 20, 19].

Very advanced calculations have been performed with improved algebraic reduction methods based on Feynman-diagrammatic algorithms, as well as with new numerical techniques based on the idea of reconstructing one-loop amplitudes from their unitarity cuts. These theoretical developments found an ideal counterpart in the integrand-level reduction algorithm, that allows for the reduction of any scattering amplitudes to scalar master integrals, simply by evaluating numerically the integrand at given fixed values of the integration momentum. In both scenarios, to tackle the increase in the complexity and in the number of diagrams that contribute to the amplitudes, automation becomes indispensable for processes with many external legs.

The purpose of the present document is to illustrate the main features of GoSam [12], a new framework which allows the automated calculation of one-loop scattering amplitudes for multi-particle processes. This approach combines the automated algebraic generation of $d$-dimensional unintegrated amplitudes obtained via Feynman diagrams, with the numerical integrand-level reduction provided by the $d$-dimensional extension [119, 120, 6] of the OPP integrand-level reduction method [121, 122, 123] and improved tensorial techniques [124, 125].

The integrands of the one-loop amplitudes are generated via Feynman diagrams, using QGRAF [126], FORM [127], spinney [128] and haggies [129]. The only task required from the user is the preparation of an "input card" to start the generation of the source code and its compilation, without having to worry about internal details of the code generation. The individual program tasks are efficiently managed by python scripts. Concerning the reduction, the program offers the possibility to use either the $d$-dimensional extension of the OPP method, as implemented in SAMURAI [6], or tensor reduction as implemented in Golem95C [130, 131] interfaced through tensorial reconstruction at the integrand level [124].

### 2.2 Algebraic approach to Automation

There are several approaches to the automated computation of multi-particle scattering amplitudes at the one-loop level, which provide different recipes for the construction of multi-purpose tools. The goal of such tools is the evaluation of one-loop scattering amplitudes for any choice of particles in the initial and final states, in a fully automated manner.

In the algebraic approach to multi-purpose automation, amplitudes can be generated from Feynman diagrams by employing tools for algebraic manipulation: already some time ago, the idea of automating NLO calculations has been pursued by public programs like FeynArts [132] and QGRAF [126] for diagram generation and FormCalc/LoopTools [133] and GRACE [3] for the automated calculation of NLO corrections, primarily in the electroweak sector.

When we combine the algebraic generation with the integrand-level reduction, the set of algebraic operations required are quite different with respect to a traditional tensorial reduction. Since the target is to provide the numerical value of the numerator function at given values of integration momentum, we should aim at expressions for the unintegrated numerator that are easily evaluated numerically. To achieve this task, for example, expressions in terms of spinor products are particularly convenient.

We briefly list here some of the advantages of the "algebraic approach": i) the algebraic generation is executed separately from the numerical reduction, therefore algebraic manipulations are possible before starting the numerical integration; CPU-time can be spent, once for all at the beginning of the calculation, to optimize and reduce the size of the integrands that will be evaluated numerically several times
later on during the reduction; ii) the algebraic method allows us to group sets of diagrams and cache all factors that do not depend on the integration momentum; iii) easy access to sub-parts of the computation; subsets of diagrams can be easily added or removed from the final results, simplifying comparisons and tests; iv) computer algebra can be performed in dimension $d$ using alternative regularization schemes; v) the choice between different reduction algorithms can be performed at run-time, providing flexibility and internal cross-checks. In the next section we will briefly illustrate how these properties are used within GoSAM.

Important progress in a similar direction has been also recently achieved by means of FeynArts, FormCalc and LoopTools [134, 2] to provide amplitudes that can be processed using the integrand-level reduction provided by CutTools [135] and/or SAMURAI [6] or with the traditional Passarino-Veltman reduction [112].

### 2.3 A brief introduction to GoSAM

GoSAM produces in a fully automated way all the code required to perform the calculation of virtual one-loop amplitudes. The only task left to the user is the preparation of an "input card" which contains all the information related to the particular process namely initial and final particles, model, helicities, selection rules to exclude particular sets of diagrams, regularization scheme. The card also contains flags to select the preferred reduction methods and some optimization flags to adapt the diagram generation to the needs of the user.

There are three main steps that GoSAM follows in order to prepare the code for the calculation: the generation of diagrams that contribute to the process, the optimization and algebraic manipulation to simplify their expressions, and the writing of a FORTRAN code ready to be used within a phase-space integration. It is important to remember that these steps will only be performed once. After the code is generated, the reduction of unintegrated amplitudes to linear combinations of scalar (master) integrals is fully embedded in the process and can be performed with different options, all available at run-time. Only the last part, namely the reduction and evaluation of master integrals, will be repeated for all the different phase-space points that contribute to the cross-section.

### 2.31 Diagram Generation

For the diagram generation both at tree level and one-loop level we employ QGRAF [126] which we complemented by adding another filter over diagrams implemented in Python. This gives several advantages since it increases the ability of the code to distinguish certain classes of diagrams and group them according to the sets of their propagators, in order to fully optimize the reduction.

At this stage GoSAm generates three sets of output files: an expression for each diagram for FORM [127], Python code for drawing each diagram, and Python code for computing the properties of the diagram. Information about the model is either read from the built-in Standard Model of QGRAF or can be defined by the user by means of LanHEP [136] or an Universal FeynRules Output (UFO) file [137]

The Python program automatically performs several operations: diagrams whose color factor turns out to be zero are dropped; the number of propagators containing the loop momentum, the tensor rank and the kinematic invariants of the associated loop integral are computed; diagrams with a vanishing loop integral associated are detected and flagged for the diagram selection; all propagators and vertices are classified for the diagram selection; diagrams containing massive quark self-energy insertions or closed massless quark loops are specially flagged.

During this phase, GoSAM also generates a ETEX file which contains, among other useful information of the generated process, the drawings of all contributing diagrams. To achieve this task, we use our own implementation of the algorithms described in Ref. [138] and Axodraw [139] to actually draw the diagrams.

### 2.32 Lorentz Algebra

Concerning the algebraic operations performed by GoSAM to render the integral suitable for efficient numerical evaluation, one of the primary goals is to split the $(4-2 \varepsilon)$ dimensional algebra into strictly four-dimensional objects and symbols representing the higher-dimensional remainder. All external vectors (momenta and polarisation vectors) are kept in four dimensions; internal vectors, however, are kept in the $d$-dimensional vector space.

We adopt the conventions used in [128], where $\hat{k}$ denotes the four dimensional projection of an in general $d$ dimensional vector $k$. The $(d-4)$ dimensional orthogonal projection is denoted as $\tilde{k}$. For the integration momentum $q$ we introduce in addition the symbol $\mu^{2}=-\tilde{q}^{2}$, such that

$$
\begin{equation*}
q^{2}=\hat{q}^{2}+\tilde{q}^{2}=\hat{q}^{2}-\mu^{2} . \tag{14}
\end{equation*}
$$

We also introduce suitable projectors by splitting the metric tensor

$$
\begin{equation*}
g^{\mu \nu}=\hat{g}^{\mu \nu}+\tilde{g}^{\mu \nu}, \quad \hat{g}^{\mu \nu} \tilde{g}_{\nu \rho}=0, \quad \hat{g}_{\mu}^{\mu}=4, \quad \tilde{g}_{\mu}^{\mu}=d-4 \tag{15}
\end{equation*}
$$

Once all propagators and all vertices have been replaced by their corresponding expressions, according to the model file, all vector-like quantities and metric tensors are split into their four-dimensional and their orthogonal part. As we use the 't Hooft algebra, $\gamma_{5}$ is defined as a purely four-dimensional object, $\gamma_{5}=i \epsilon_{\mu \nu \rho \sigma} \hat{\gamma}^{\mu} \hat{\gamma}^{\nu} \hat{\gamma}^{\rho} \hat{\gamma}^{\sigma}$. By applying the usual anti-commutation relation for Dirac matrices we can always separate the four-dimensional and $(d-4)$-dimensional parts of Dirac traces.

While the $(d-4)$-dimensional traces are reduced completely to products of $(d-4)$-dimensional metric tensors, the four-dimensional part, which will be reduced numerically, is treated such that the number of terms in the resulting expression is kept as small as possible.

### 2.33 Treatment of rational terms $R_{2}$

Instead of relying on the construction of $R_{2}$ from specialized Feynman rules [123, 140, 141, 142, 143], we can generate the $R_{2}$ part along with all other contribution using automated algebraic manipulations. The code offers the option between the implicit and explicit construction of the $R_{2}$ terms. The implicit construction treats the $4-$ and $(d-4)$ dimensional numerators on equal grounds: they are generated algebraically and reduced numerically. The explicit construction of $R_{2}$ is based on the fact that the $(d-4)$ dimensional part of the numerator function contains expressions for the corresponding integrals that are relatively simple and known explicitly. Therefore, after separating it using the algebraic manipulation described before, the $(d-4)$ dimensional part is computed analytically whereas the purely four-dimensional part is passed to the numerical reduction. This approach also allows for an efficient calculation of the part $R_{2}$ alone.

### 2.34 Reduction to scalar (master) integrals

GoSAM allows to choose at run-time (i.e. without re-generating the code) the preferred method of reduction. Available options include the integral-level $d$-dimensional reduction, as implemented in SAMURAI, or traditional tensor reduction as implemented in Golem95C interfaced through tensorial reconstruction at the integrand level, or a combination of both. Concerning the scalar (tensorial) integrals, GoSAM allows to choose among a variety of options, including QCDLoop [109], OneLoop [111], Golem95C [130], plus the recently added P JFRY [108]. Among these codes, OneLoop and Golem95C also fully support complex masses.

### 2.4 Installation and Usage

GoSam can be used within a standard Linux/Unix environment. In order to work, it requires some programs to be installed on the system: these include a recent version of Python (version $\geq 2.6$ ), Java
( $\geq 1.5$ ), a Fortran 95 compiler, FORM (version $\geq 3.3$ ), and QGRAF. Further, at least one of the libraries SAMURAI or Golem95C needs to be present at the time the code is compiled.

To facilitate this task, we have prepared a package containing SAMURAI and Golem95C together with the libraries for the integrals: OneLOop, QCDLoop, and FF. The package, which is called gosam-contrib-1.0.tar.gz is available for download from

```
http://projects.hepforge.org/gosam/.
```

The installation procedure is facilitated by the use of Autotools.
The user can download the GoSAM code either as a tar-ball or from the subversion repository at http://projects.hepforge.org/gosam/. The installation of GoSam is controlled by Python Distutils and can be performed by simply running the command

```
python setup.py install
```

In order to generate the code for a process, the user needs to prepare an input file (process card) which contains:

- process specific information, such as a list of initial and final state particles, their helicities (optional) and the order of the coupling constants;
- scheme specific information, such as the regularisation and renormalisation schemes, the underlying model, masses and widths which are set to zero;
- system specific information, such as paths to programs and libraries or compiler options;
- optional information for optimisations within the code generation.

Assuming that the process card is called myprocess.in, the generation of the code can be started by simply running the command gosam.py myprocess.in. All further steps are controlled by makefiles which are automatically generated by GoSAM: the command make compile generates the source code and compiles all files relevant for the production of the matrix element. The code can be tested with the program test. f 90 (located in the subdirectory matrix) which provides, for a random phase-space point, the tree-level LO matrix element and the NLO result for the finite part, single and double poles. Examples of process cards for a selection of benchmark processes are provided with the main distubution.

For more details about the usage and installation of GoSAM, we refer the user to a more technical presentation [144] or to the original publication [12] and the user manual which accompanies the code.

### 2.5 Examples of Applications

The BLHA interface [145] allows to link GoSAM to a general Monte Carlo event generator, which is responsible for supplying the missing ingredients for a complete NLO calculation of a physical cross section. Among those, SHERPA [146] offers the possibility to compute the LO cross section and the real corrections with both the subtraction terms and the corresponding integrated counterparts [147]. Using the BLHA interface, we linked GoSAM with SHERPA to compute the physical cross section for $W^{ \pm}+1$-jet at NLO, which is described in Section 18 .

The codes produced by GoSam have been tested on several processes of increasing complexity, some of which are shown in Table 1. The full list of processes produced by GoSam and compared to the literature where available is given in Ref. [12].

As an example of the usage of GoSam with a model file different from the Standard Model, we calculated the QCD corrections to neutralino pair production in the MSSM. The model file has been imported using the UFO interface. In this calculation, we combined the one-loop amplitude with the real radiation corrections to obtain results for differential cross sections. For the infrared subtraction terms

| $e^{+} e^{-} \rightarrow u \bar{u}$ | $[148]$ |
| :--- | :--- |
| $e^{+} e^{-} \rightarrow t \bar{t}$ | $[149,150]$, own analytic calculation |
| $u \bar{u} \rightarrow d \bar{d}$ | $[15$, 8] |
| $g g \rightarrow g g$ | $[152]$ |
| $g g \rightarrow g Z$ | $[153]$ |
| $b g \rightarrow H b$ | $[154,8]$ |
| $\gamma \gamma \rightarrow \gamma \gamma(\mathrm{W}$ loop) | $[15]$ |
| $\gamma \gamma \rightarrow \gamma \gamma \gamma \gamma$ (fermion loop) | $[156]$ |
| $p p \rightarrow t \bar{t}$ | $[8]$, MCFM [157, 158] |
| $p p \rightarrow W^{ \pm} j$ (QCD corr.) | $[157,158]$ |
| $p p \rightarrow W^{ \pm} j$ (EW corr.) | for IR poles: [65, 159] |
| $p p \rightarrow W^{ \pm} t$ | $[157,158]$ |
| $p p \rightarrow W^{ \pm} j j$ | $[157,158]$ |
| $p p \rightarrow W^{ \pm} b \bar{b}$ (massive b) | $[157,158$ |
| $e^{+} e^{-} \rightarrow e^{+} e^{-} \gamma(\mathrm{QED})$ | $[160]$ |
| $p p \rightarrow H t t \bar{t}$ | $[8]$ |
| $p p \rightarrow Z t \bar{t}$ | $[10]$ |
| $p p \rightarrow W^{+} W^{+} j j$ | $[56$, v3] |
| $p p \rightarrow b \bar{b} b \bar{b}$ | $[62,63]$ |
| $p p \rightarrow W^{+} W^{-} b \bar{b}$ | $[8,161]$ |
| $p p \rightarrow t \bar{t} b \bar{b}$ | $[8,161]$ |
| $u \bar{d} \rightarrow W^{+} g g g$ | $[161]$ |

Table 3: Some of the processes computed and checked with GoSAm
we employed MadDipole [162], while the real emission part is calculated using MadGraph/MadEvent [163]. The virtual matrix element is renormalized in the $\overline{M S}$ scheme, while massive particles are treated in the on-shell scheme. The renormalization terms specific to the massive MSSM particles have been added manually. In Fig $\sqrt[4]{ }$ we show the differential cross section for the $m_{\chi_{1}^{0} \chi_{1}^{0}}$ invariant mass, where we employed a jet veto to suppress large contributions from the channel $q g \rightarrow \chi_{1}^{0} \chi_{1}^{0} q$ which opens up at order $\alpha^{2} \alpha_{s}$, but for large $p_{T}^{j e t}$ belongs to the distinct process of neutralino pair plus one hard jet production at leading order.


Fig. 4: Comparison of the NLO and LO $m_{\chi_{1}^{0} \chi_{1}^{0}}$ distributions for the process $p p \rightarrow \chi_{1}^{0} \chi_{1}^{0}$ with a jet veto on jets with $p_{T}^{j e t}>20 \mathrm{GeV}$ and $\eta<4.5$. The band gives the dependence of the result on $\mu=\mu_{F}=\mu_{R}$ between $\mu_{0} / 2$ and $2 \mu_{0}$. We choose $\mu_{0}=m_{Z}$.

## Conclusions and Outlook

Several groups are currently working at the development of automated multi-purpose tools for one-loop calculations. For quite a long time, tree-level calculation have been fully automated and included in flexible multi-process tools [164, 165]. The level of automation achieved by one-loop calculations is suggesting the possibility of a similar success also at the next-lo-leading order. The target is to build efficient and flexible NLO programs which can be used to tackle the increasing need of precision required by the experimental collaborations.

GoSam is a flexible and broadly applicable tool for the fully automated evaluation of one-loop scattering amplitudes. In this approach, scattering amplitudes are generated in terms of Feynman diagrams and their reduction to master integrals can be performed in several ways, which can be selected at run-time. GoSAm can be used to calculate one-loop corrections both in QCD and electro-weak theory and offers the flexibility to link general model files for theories Beyond the Standard Model. The code performed well in reproducing a wide range of examples and we are looking forward to tackle more challenging calculations and interfacing with other existing tools in the near future.

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## 3. AUTOMATION AND NUMERICAL LOOP INTEGRATION ${ }^{5}$

### 3.1 INTRODUCTION

Numerical methods are nowadays routinely used in fully differential fixed-order perturbative calculations for the integration over the phase-space of the final-state particles. The use of numerical methods for the phase-space integration allows the flexibility to compute any infrared-safe observable for a given process within a single numerical program. It is thus natural to investigate if numerical methods can also be applied for the loop integration in the virtual corrections [166, 167, $168,169,170,171,172,173$ [174, 175, 176]. A major breakthrough was achieved recently by showing that the numerical method is compatible in efficency with the commonly used approaches based on cut techniques and generalised unitarity or on Feynman graphs [70, [51, 53, 22, 20, 52, 117, 56, 54, 50, 48, 177, 111, 5, 178, 8, 12]. The implementation of the numerical method for the loop integration is process-independent and offers therefore the flexibility to compute several processes within one numerical program. We discuss the main principles of the numerical method for the loop integration at one-loop. In addition we give an outlook towards higher loops.

### 3.2 THE SUBTRACTION METHOD FOR THE LOOP INTEGRATION

The contributions to an infrared-safe $n$-jet observable observable $O$ at next-to-leading order are given by

$$
\begin{equation*}
\langle O\rangle^{N L O}=\int_{n+1} O_{n+1} d \sigma^{R}+\int_{n} O_{n} d \sigma^{V}+\int_{n} O_{n} d \sigma^{C} . \tag{16}
\end{equation*}
$$

[^119]Here a rather condensed notation is used. $d \sigma^{R}$ denotes the real emission contribution, whose matrix elements are given by the square of the Born amplitudes with $(n+3)$ partons $\left|A_{n+3}^{(0)}\right|^{2} . d \sigma^{V}$ denotes the virtual contribution, whose matrix elements are given by the interference term of the one-loop and Born amplitude $\operatorname{Re}\left(A_{n+2}^{(0)^{*}} A_{n+2}^{(1)}\right)$ and $d \sigma^{C}$ denotes a collinear subtraction term, which subtracts the initial state collinear singularities. Each term is separately divergent and only their sum is finite.

The subtraction method is widely used to render the real emission part of a NLO calculation suitable for a numerical Monte Carlo integration. One adds and subtracts a suitably chosen piece to be able to perform the phase-space integrations by Monte Carlo methods:

$$
\begin{equation*}
\langle O\rangle^{N L O}=\int_{n+1}\left(O_{n+1} d \sigma^{R}-O_{n} d \sigma^{A}\right)+\int_{n}\left(O_{n} d \sigma^{V}+O_{n} d \sigma^{C}+O_{n} \int_{1} d \sigma^{A}\right) . \tag{17}
\end{equation*}
$$

The first term $\left(O_{n+1} d \sigma^{R}-O_{n} d \sigma^{A}\right)$ is by construction integrable over the $(n+1)$-particle phase-space and can be evaluated numerically. The result of the integration of the subtraction term over the unresolved one-parton phase-space is written in a compact notation as

$$
\begin{equation*}
d \sigma^{C}+\int_{1} d \sigma^{A}=(\mathbf{I}+\mathbf{K}+\mathbf{P}) \otimes d \sigma^{B} \tag{18}
\end{equation*}
$$

The notation $\otimes$ indicates that colour correlations due to the colour charge operators $\mathbf{T}_{i}$ still remain. The terms with the insertion operators $\mathbf{K}$ and $\mathbf{P}$ pose no problem for a numerical evaluation. The term $\mathbf{I} \otimes d \sigma^{B}$ lives on the phase-space of the $n$-parton configuration and has the appropriate singularity structure to cancel the infrared divergences coming from the one-loop amplitude. Therefore $d \sigma^{V}+\mathbf{I} \otimes d \sigma^{B}$ is infrared finite.

We extend this subtraction method to the virtual part such that we can evaluate the one-loop integral of the one-loop amplitude numerically. The renormalised one-loop amplitude $\mathcal{A}^{(1)}$ is related to the bare amplitude $\mathcal{A}_{\text {bare }}^{(1)}$ by $\mathcal{A}^{(1)}=\mathcal{A}_{\mathrm{bare}}^{(1)}+\mathcal{A}_{\mathrm{CT}}^{(1)}$, where $\mathcal{A}_{\mathrm{CT}}^{(1)}$ denotes the ultraviolet counterterm from renormalisation. The bare amplitude involves the loop integration

$$
\begin{equation*}
\mathcal{A}_{\mathrm{bare}}^{(1)}=\int \frac{d^{D} k}{(2 \pi)^{D}} \mathcal{G}_{\mathrm{bare}}^{(1)} . \tag{19}
\end{equation*}
$$

where $\mathcal{G}_{\text {bare }}^{(1)}$ denotes the integrand of the bare one-loop amplitude. We introduce subtraction terms which match locally the singular behaviour of the bare integrand:

$$
\begin{equation*}
\mathcal{A}_{\text {bare }}^{(1)}+\mathcal{A}_{\mathrm{CT}}^{(1)}=\int \frac{d^{D} k}{(2 \pi)^{D}}\left(\mathcal{G}_{\text {bare }}^{(1)}-\mathcal{G}_{\mathrm{soft}}^{(1)}-\mathcal{G}_{\mathrm{coll}}^{(1)}-\mathcal{G}_{\mathrm{UV}}^{(1)}\right)+\left(\mathcal{A}_{\mathrm{CT}}^{(1)}+\mathcal{A}_{\mathrm{soft}}^{(1)}+\mathcal{A}_{\text {coll }}^{(1)}+\mathcal{A}_{\mathrm{UV}}^{(1)}\right) . \tag{20}
\end{equation*}
$$

Analogous to $\mathcal{G}_{\text {bare }}^{(1)}$, the integrands of the subtraction terms $\mathcal{A}_{x}^{(1)}$ are denoted by $\mathcal{G}_{x}^{(1)}$, where $x$ is equal to soft, coll or UV. The expression in the first bracket is finite and can therefore be integrated numerically in four dimensions. The integrated subtraction terms in the second bracket are easily calculated analytically in $D$ dimensions. The result can be written as

$$
\begin{equation*}
2 \operatorname{Re} \mathcal{A}^{(0)}\left(\mathcal{A}_{\mathrm{CT}}^{(1)}+\mathcal{A}_{\mathrm{soft}}^{(1)}+\mathcal{A}_{\mathrm{coll}}^{(1)}+\mathcal{A}_{\mathrm{UV}}^{(1)}\right)^{*} O_{n} d \phi_{n}=\mathbf{L} \otimes d \sigma^{B} . \tag{21}
\end{equation*}
$$

The insertion operator $\mathbf{L}$ contains the explicit poles in the dimensional regularisation parameter related to the infrared singularities of the one-loop amplitude. These poles cancel when combined with the insertion operator $\mathbf{I}$ :

$$
\begin{equation*}
(\mathbf{I}+\mathbf{L}) \otimes d \sigma^{B}=\text { finite } \tag{22}
\end{equation*}
$$

The operator $\mathbf{L}$ contains, as does the operator $\mathbf{I}$, colour correlations due to soft gluons. In analogy to the one-loop amplitude we can write $d \sigma^{V}=d \sigma_{\mathrm{CT}}+\int \frac{d^{D} k}{(2 \pi)^{D}} d \sigma_{\text {bare }}^{V}$ and then the NLO contributions reads

$$
\begin{align*}
& \langle O\rangle^{N L O}=  \tag{23}\\
& \quad \int_{n+1}\left(O_{n+1} d \sigma^{R}-O_{n} d \sigma^{A}\right)+\int_{n+\text { loop }} O_{n}\left(d \sigma_{\text {bare }}^{V}-d \sigma^{A^{\prime}}\right)+\int_{n} O_{n}(\mathbf{I}+\mathbf{L}+\mathbf{K}+\mathbf{P}) \otimes d \sigma^{B} .
\end{align*}
$$

In a condensed notation this reads

$$
\begin{equation*}
\langle O\rangle^{N L O}=\langle O\rangle_{\text {real }}^{N L O}+\langle O\rangle_{\text {virtual }}^{N L O}+\langle O\rangle_{\text {insertion }}^{N L O} . \tag{24}
\end{equation*}
$$

Every single term is finite and can be evaluated numerically.

### 3.3 THE SUBTRACTION TERMS

Amplitudes in QCD may be decomposed into group-theoretical factors (carrying the colour structures) multiplied by kinematic factors called partial amplitudes. At the loop level partial amplitudes may further be decomposed into primitive amplitudes. It is simpler to work with primitive one-loop amplitudes instead of a full one-loop amplitude. Our method exploits the fact that primitive one-loop amplitudes have a fixed cyclic ordering of the external legs and that they are gauge-invariant. The first point ensures that there are at maximum $n$ different loop propagators in the problem, where $n$ is the number of external legs, while the second property of gauge invariance is crucial for the proof of the method. We therefore consider in the following just a single primitive one-loop amplitude, which we denote by $A^{(1)}$, while keeping in mind that the full one-loop amplitude is just the sum of several primitive amplitudes multiplied by colour structures. We label the external momenta clockwise by $p_{1}, p_{2}, \ldots, p_{n}$ and define $q_{i}=p_{1}+$ $p_{2}+\ldots+p_{i}, k_{i}=k-q_{i}$. We can write the bare primitive one-loop amplitude in Feynman gauge as

$$
\begin{equation*}
A_{\text {bare }}^{(1)}=\int \frac{d^{D} k}{(2 \pi)^{D}} G_{\text {bare }}^{(1)}, \quad G_{\text {bare }}^{(1)}=P(k) \prod_{i=1}^{n} \frac{1}{k_{i}^{2}-m_{i}^{2}+i \delta} . \tag{25}
\end{equation*}
$$

$G_{b a r e}^{(1)}$ is the integrand of the bare one-loop amplitude. $P(k)$ is a polynomial in the loop momentum $k$. The $+i \delta$-prescription instructs us to deform - if possible - the integration contour into the complex plane to avoid the poles at $k_{i}^{2}=m_{i}^{2}$. If a deformation close to a pole is not possible, we say that the contour is pinched. If we restrict ourselves to non-exceptional external momenta, then the divergences of the one-loop amplitude related to a pinched contour are either due to soft or collinear partons in the loop. These divergences are regulated within dimensional regularisation by setting the number of space-time dimensions equal to $D=4-2 \varepsilon$. A primitive amplitude which has soft or collinear divergences must have at least one loop propagator which corresponds to a gluon. An amplitude which just consists of a closed fermion loop does not have any infrared divergences. We denote by $I_{g}$ the set of indices $i$, for which the propagator $i$ in the loop corresponds to a gluon. The soft and collinear subtraction terms for massless QCD read [169]

$$
\begin{align*}
G_{\mathrm{soft}}^{(1)} & =16 \pi \alpha_{s} i \sum_{j \in I_{g}} \frac{p_{j} \cdot p_{j+1}}{k_{j-1}^{2} k_{j}^{2} k_{j+1}^{2}} A_{j}^{(0)}, \\
G_{\mathrm{coll}}^{(1)} & =-8 \pi \alpha_{s} i \sum_{j \in I_{g}}\left[\frac{S_{j} g_{\mathrm{UV}}\left(k_{j-1}^{2}, k_{j}^{2}\right)}{k_{j-1}^{2} k_{j}^{2}}+\frac{S_{j+1} g_{\mathrm{UV}}\left(k_{j}^{2}, k_{j+1}^{2}\right)}{k_{j}^{2} k_{j+1}^{2}}\right] A_{j}^{(0)}, \tag{26}
\end{align*}
$$

where $S_{j}=1$ if the external line $j$ corresponds to a quark and $S_{j}=1 / 2$ if it corresponds to a gluon. The function $g_{\mathrm{UV}}$ ensures that the integration over the loop momentum is ultraviolet finite. Integrating
the soft and the collinear part we obtain

$$
\begin{align*}
& S_{\varepsilon}^{-1} \mu_{s}^{2 \varepsilon} \int \frac{d^{D} k}{(2 \pi)^{D}} G_{\mathrm{soft}}^{(1)}=-\frac{\alpha_{s}}{4 \pi} \frac{e^{\varepsilon \gamma_{E}}}{\Gamma(1-\varepsilon)} \sum_{j \in I_{g}} \frac{2}{\varepsilon^{2}}\left(\frac{-2 p_{j} p_{j+1}}{\mu_{s}^{2}}\right)^{-\varepsilon} A_{j}^{(0)}+\mathcal{O}(\varepsilon) \\
& S_{\varepsilon}^{-1} \mu_{s}^{2 \varepsilon} \int \frac{d^{D} k}{(2 \pi)^{D}} G_{\mathrm{coll}}^{(1)}=-\frac{\alpha_{s}}{4 \pi} \frac{e^{\varepsilon \gamma_{E}}}{\Gamma(1-\varepsilon)} \sum_{j \in I_{g}}\left(S_{j}+S_{j+1}\right) \frac{2}{\varepsilon}\left(\frac{\mu_{u v}^{2}}{\mu_{s}^{2}}\right)^{-\varepsilon} A_{j}^{(0)}+\mathcal{O}(\varepsilon) \tag{27}
\end{align*}
$$

$S_{\varepsilon}=(4 \pi)^{\varepsilon} e^{-\varepsilon \gamma_{E}}$ is the typical volume factor of dimensional regularisation, $\gamma_{E}$ is Euler's constant and $\mu$ is the renormalisation scale.

The ultraviolet subtraction terms correspond to propagator and vertex corrections. The subtraction terms are obtained by expanding the relevant loop propagators around a new ultraviolet propagator $\left(\bar{k}^{2}-\right.$ $\left.\mu_{\mathrm{UV}}^{2}\right)^{-1}$, where $\bar{k}=k-Q$ : For a single propagator we have

$$
\frac{1}{(k-p)^{2}}=\frac{1}{\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}}+\frac{2 \bar{k} \cdot(p-Q)}{\left(\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}\right)^{2}}-\frac{(p-Q)^{2}+\mu_{\mathrm{UV}}^{2}}{\left(\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}\right)^{2}}+\frac{[2 \bar{k} \cdot(p-Q)]^{2}}{\left(\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}\right)^{3}}+\mathcal{O}\left(\frac{1}{|\bar{k}|^{5}}\right)
$$

We can always add finite terms to the subtraction terms. For the ultraviolet subtraction terms we choose the finite terms such that the finite parts of the integrated ultraviolet subtraction terms are independent of $Q$ and proportional to the pole part, with the same constant of proportionality for all ultraviolet subtraction terms. This ensures that the sum of all integrated UV subtraction terms is again proportional to a tree-level amplitude [167].

### 3.4 CONTOUR DEFORMATION

Having a complete list of ultraviolet and infrared subtraction terms at hand, we can ensure that the integration over the loop momentum gives a finite result and can therefore be performed in four dimensions. However, this does not yet imply that we can safely integrate each of the four components of the loop momentum $k^{\mu}$ from minus infinity to plus infinity along the real axis. There is still the possibility that some of the loop propagators go on-shell for real values of the loop momentum. If the contour is not pinched this is harmless, as we may escape into the complex plane in a direction indicated by Feynman's $+i \delta$-prescription. However, it implies that the integration should be done over a region of real dimension 4 in the complex space $\mathbb{C}^{4}$. Let us consider an integral corresponding to a primitive one-loop amplitude with $n$ propagators minus the appropriate IR- and UV-subtraction terms:

$$
\begin{equation*}
\int \frac{d^{4} \tilde{k}}{(2 \pi)^{4}}\left(\mathcal{G}_{\mathrm{bare}}^{(1)}-\mathcal{G}_{\mathrm{soft}}^{(1)}-\mathcal{G}_{\mathrm{coll}}^{(1)}-\mathcal{G}_{\mathrm{UV}}^{(1)}\right)=\int \frac{d^{4} \tilde{k}}{(2 \pi)^{4}} P(\tilde{k}) \prod_{j=1}^{n} \frac{1}{\tilde{k}_{j}^{2}-m_{j}^{2}+i \delta} \tag{28}
\end{equation*}
$$

where $P(\tilde{k})$ is a polynomial of the loop momentum $\tilde{k}^{\mu}$ and the integration is over a complex contour in order to avoid whenever possible the poles of the propagators. We set $\tilde{k}^{\mu}=k^{\mu}+i \kappa^{\mu}(k)$, where $k^{\mu}$ is real [170]. After this deformation our integral equals

$$
\begin{equation*}
\int \frac{d^{4} k}{(2 \pi)^{4}}\left|\frac{\partial \tilde{k}^{\mu}}{\partial k^{\nu}}\right| P(\tilde{k}(k)) \prod_{j=1}^{n} \frac{1}{k_{j}^{2}-m_{j}^{2}-\kappa^{2}+2 i k_{j} \cdot \kappa} \tag{29}
\end{equation*}
$$

To match Feynman's $+i \delta$-prescription we have to construct the deformation vector $\kappa$ such that

$$
\begin{equation*}
k_{j}^{2}-m_{j}^{2}=0 \quad \rightarrow \quad k_{j} \cdot \kappa \geq 0 \tag{30}
\end{equation*}
$$

We remark that the numerical stability of the Monte Carlo integration depends strongly on the definition of the deformation vector $\kappa$.

### 3.5 NLO results for $\mathbf{n}$-jets in electron-positron annihilation

We have calculated results for jet observables in electron-positron annihilation, where the jets are defined by the Durham jet algorithm [166]. The cross section for $n$ jets normalised to the LO cross section for $e^{+} e^{-} \rightarrow$ hadrons reads

$$
\begin{equation*}
\frac{\sigma_{n-j e t}(\mu)}{\sigma_{0}(\mu)}=\left(\frac{\alpha_{s}(\mu)}{2 \pi}\right)^{n-2} A_{n}(\mu)+\left(\frac{\alpha_{s}(\mu)}{2 \pi}\right)^{n-1} B_{n}(\mu)+\mathcal{O}\left(\alpha_{s}^{n}\right) . \tag{31}
\end{equation*}
$$

One can expand the perturbative coefficient $A_{n}$ and $B_{n}$ in $1 / N_{c}$ :

$$
A_{n}=N_{c}\left(\frac{N_{c}}{2}\right)^{n-2}\left[A_{n, \mathrm{lc}}+\mathcal{O}\left(\frac{1}{N_{c}}\right)\right], \quad B_{n}=N_{c}\left(\frac{N_{c}}{2}\right)^{n-1}\left[B_{n, \mathrm{lc}}+\mathcal{O}\left(\frac{1}{N_{c}}\right)\right] .
$$

We calculate the leading order coefficient $A_{n, \text { lc }}$ and the next-to-leading order coefficient $B_{n, \text { lc }}$ for $n \leq 7$ at the renormalisation scale $\mu$ equal to the centre-of-mass energy. The centre-of-mass energy is taken to be equal to the mass of the $Z$-boson. The scale variation can be restored from the renormalisation group equation. The calculation is done with five massless quark flavours. Fig. 5 ]shows the comparison of our




Fig. 5: Comparison of the NLO corrections to the two-, three- and four-jet rate between the numerical calculation and an analytic calculation. The error bars from the Monte Carlo integration are shown and are almost invisible.
numerical approach with the well-known results for two, three and four jets [179, 180, 181]. We observe an excellent agreement. The results for five, six and seven jets for the jet parameter $y_{c u t}=0.0006$ are

$$
\begin{array}{ll}
\frac{N_{c}^{4}}{8} A_{5, \mathrm{lc}}=(2.4764 \pm 0.0002) \cdot 10^{4}, & \frac{N_{c}^{5}}{16} B_{5, \mathrm{lc}}=(1.84 \pm 0.15) \cdot 10^{6}, \\
\frac{N_{c}^{5}}{16} A_{6, \mathrm{lc}}=(2.874 \pm 0.002) \cdot 10^{5}, & \frac{N_{c}^{6}}{32} B_{6, \mathrm{lc}}=(3.88 \pm 0.18) \cdot 10^{7}, \\
\frac{N_{c}^{6}}{32} A_{7, \mathrm{lc}}=(2.49 \pm 0.08) \cdot 10^{6}, & \frac{N_{c}^{7}}{64} B_{7, \mathrm{lc}}=(5.4 \pm 0.3) \cdot 10^{8} . \tag{32}
\end{array}
$$

### 3.6 FIRST STEPS TOWARDS NNLO

An NNLO calculation requires among other things also the calculation of the one-loop amplitude squared. The expansion in the dimensional regularisation parameter $\varepsilon$ of the one-loop amplitude starts at order $(-2)$ one would naively expect that up to order $\varepsilon^{0}$ the $\mathcal{O}(\uparrow)$ - and $\mathcal{O}\left(\varepsilon^{2}\right)$-terms of the one-loop amplitude are needed for an NNLO calculation. However, it is by no means obvious how the approaches for one-loop amplitudes based on unitarity or the numerical method can be extended to include the higherorder terms in the $\varepsilon$-expansion. It turns out that the computation of these higher-order terms can be avoided, provided a method is known to compute the finite two-loop remainder function. The one- and two-loop amplitudes can be written as [182]

$$
\begin{align*}
\mathcal{A}^{(1)} & =\mathbf{Z}^{(1)} \mathcal{A}^{(0)}+\mathcal{F}_{\text {minimal }}^{(1)}, \\
\mathcal{A}^{(2)} & =\left(\mathbf{Z}^{(2)}-\mathbf{Z}^{(1)} \mathbf{Z}^{(1)}\right) \mathcal{A}^{(0)}+\mathbf{Z}^{(1)} \mathcal{A}^{(1)}+\mathcal{F}_{\text {minimal }}^{(2)}, \tag{33}
\end{align*}
$$

where the operators $\mathbf{Z}^{(1)}$ and $\mathbf{Z}^{(2)}$ contain all the infrared poles and $\mathcal{F}_{\text {minimal }}^{(1)}$ and $\mathcal{F}_{\text {minimal }}^{(2)}$ are finite remainders. Here we used the convention that the operators $\mathbf{Z}^{(1)}$ and $\mathbf{Z}^{(2)}$ contain only pole terms, but no terms of order $\varepsilon^{k}$ with $k \geq 0$. This corresponds to a minimal scheme. The operators $\mathbf{Z}^{(1)}$ and $\mathbf{Z}^{(2)}$ are well-known. At NNLO it is sufficient to know the $\varepsilon^{0}$-terms of $\mathcal{F}_{\text {minimal }}^{(1)}$ and $\mathcal{F}_{\text {minimal }}^{(2)}$, the $\varepsilon^{1}$ - or $\varepsilon^{2}$-terms of $\mathcal{A}^{(1)}$ or $\mathcal{F}_{\text {minimal }}^{(1)}$ are not required [183].

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## 4. TOWARDS THE AUTOMATION OF ONE-LOOP AMPLITUDES ${ }^{6}$


#### Abstract

A program is presented that computes one-loop amplitudes automatically for processes with up to 6 external particles based on the Feynman-diagram approach. Additionally, universal one-loop building blocks, which can be used to compute several processes at NLO QCD are calculated.


### 4.1 INTRODUCTION

The calculation of processes with multi-particle final states beyond the leading order approximation has been an active field of research during the last years as a consequence of the demand of high accuracy for signal and background processes at the LHC. A next-to-leading (NLO) calculation consists of virtual and real radiation processes which are infrared divergent (IR) separately and can be computed numerically only after extracting the divergences of the real radiation contributions. The one-loop virtual calculation for multiple particles poseses a challenge of complexity not only due to the large number of contributing diagrams, but also concerning the stability of the numerical code to evaluate them. In the last years, an enormous progress has been achieved applying new techniques and using traditional Feynman-diagram approach, leading to new NLO predictions.

Due to the large number of processes of potential interest at the LHC, the scientific community has worked in the automation of the NLO calculations. The automation of the real contributions including their infrared subtraction terms has been successfully implemented in several packages and the automation of the virtual corrections, which is a harder problem, is currently being achieved in several programs (see [184] and references therein).

In Ref. [185], the early stage of a program, in the framework of Mathematica [186] and FeynCalc [187], to compute automatically one-loop amplitudes based on traditional Feynman-diagram techniques and involving up to $2 \rightarrow 4$ processes was presented. This program will become publicly available in the future. The method used is described in Section 4.2. In Section 4.3, we present a set of universal one-loop building blocks that has been used to compute recently several processes included in the VBFNLO package [42, 41].

### 4.2 TOWARDS AN AUTOMATIC ONE-LOOP AMPLITUDE GENERATOR

The program above mentioned automatically simplifies a set of amplitudes up to Hexagons of rank 5. The result is given in terms of scalar and tensor integrals following the Passarino-Veltman convention [112, 185], spinor chains, polarization vectors and model parameters. The simplified expression is written automatically to FORTRAN routines. For massless propagators, the amplitudes can be evaluated also in Mathematica with unlimited precision, which is used for testing purposes. To achieve that, the scalar integrals, the tensor reduction formalism to extract the tensor coefficient integrals, and also the helicity method described in Ref. [188, 189] to compute the spinor products have been implemented at

[^120]the FORTRAN and Mathematica level. For the determination of the tensor integrals up to the box level, the Passarino-Veltman tensor reduction formalism [112] is used applying the LU decomposition method to avoid the explicit calculation of inverse Gram matrices by solving a system of linear equations, which is a more stable procedure close to singular points. Finally, for singular Gram determinants, special tensor reduction routines following Ref. [115] have been implemented, however, the external momenta convention (Passarino-like) was used. The impact of these methods is discussed in detail in Ref. [185]. For pentagons, in addition to the Passarino-Veltman formalism, the method proposed by Denner and Dittmaier [115, 190], applied also to hexagons, has been implemented. For that, the recursion relations of Ref. [115] in terms of the Passarino-Veltman external momenta convention have been re-derived. This last method is used for the numerical implementation at the FORTRAN level.

The Mathematica function does several algebraic manipulations that are summarized as follows:

- Simultaneous extraction of rational terms based on Dirac algebra manipulations and cancelation of scalar products against propagators.
- Reduction to a minimal basis of tensor and scalar integrals.
- Reduction to a minimal basis of spinor chains.
- The use of Chisholm identities, which are only valid in 4 dimensions, for the contraction of Lorentz indices among different spinor chains is applied, if selected.
- Factorization of loop dependent and independent factors (Useful to perform gauge tests, Ward identities or the re-evaluation of the amplitudes for different helicity polarization of gluons and fermions at a lower CPU cost).
As an example of the notation used, the following Hexagon diagram is used. This is written as follows:

where $g_{0}$ is the strong unrenormalized coupling, $\mathcal{C}_{i j}^{V_{1} V_{2} V_{3} V_{4}}$ is a color diagram dependent factor, e.g, $\mathcal{C}_{i j}^{\gamma \gamma g \gamma}=\left(T_{a}\right)_{i j}\left(C_{F}-1 / 2 C_{A}\right) . g_{\tau}^{V_{i} f}$ are electroweak couplings and $\mathcal{M}_{\tau}^{i j}$ represents the amplitude considering generic off-shell vector bosons with color indices $i j$ for a given helicity $\tau$. The amplitude $\mathcal{M}_{\tau}^{i j}$, omitting color indices, is written in terms of

$$
\begin{equation*}
\mathcal{M}_{\tau}=\mathcal{M}_{\tau}^{D=4}+(D-4) \mathcal{M}_{\tau}^{D R} \tag{35}
\end{equation*}
$$

where $\mathcal{M}_{\tau}^{D=4}$ is the amplitude that one would obtain performing the Dirac algebra manipulation in four dimensions, $D=4$, and $\mathcal{M}_{\tau}^{D R}$ contains the rational terms and vanishes in Dimensional Reduction $(D R)$. These functions are decomposed in the form:

$$
\begin{equation*}
\mathcal{M}^{(D=4, D R)}=\sum_{i, j} \mathrm{SM}_{i, \tau} \mathrm{Fl}_{j}, \tag{36}
\end{equation*}
$$

where $\mathrm{SM}_{i, \tau}$ is a basis of Standard Matrix elements corresponding to spinor products describing the quark line of Eq. (34] which are computed following the helicity method [188, 189] with a defined helicity, $\tau . \mathrm{F1}_{j}$ are complex functions which are further decomposed into dependent and independent loop integral parts,

$$
\begin{equation*}
\mathrm{F}_{j}=\sum_{l, k} \mathrm{~F}_{l} T_{k}\left(\epsilon\left(p_{n}\right) \cdot p_{m} ; \epsilon\left(p_{i}\right) \cdot \epsilon\left(p_{r}\right)\right) \tag{37}
\end{equation*}
$$

$T_{k}$ is a monomial function at most for each polarization vector $\epsilon\left(p_{x}\right)$, i.e., $\epsilon\left(p_{x}\right)^{0}$ or $\epsilon\left(p_{x}\right)^{1}$. The first possibility, $\epsilon\left(p_{x}\right)^{0}$, implies that the polarization vector appears in the set of Standard Matrix elements
$\mathrm{SM}_{i, \tau} . F_{l}$ contains kinematic variables $\left(p_{i} \cdot p_{j}\right)$, the scalar integrals ( $B_{0}, C_{0}, D_{0}$ ), and the tensor integral coefficients $\left(B_{i j}, C_{i j}, D_{i j}, E_{i j}, F_{i j}\right)$. Then, the full result is obtained from $\mathcal{M}_{\tau}^{D=4}$ and $\mathcal{M}_{\tau}^{D R}$ using the finite and the coefficients of the $1 / \epsilon^{n}$ poles of the scalar and tensor coefficient integrals:

$$
\begin{equation*}
\mathcal{M}_{v}^{D=4}=\widetilde{\mathcal{M}}_{v}+\frac{\mathcal{M}_{v}^{1}}{\epsilon}+\frac{\mathcal{M}_{v}^{2}}{\epsilon^{2}}, \quad(D-4) \mathcal{M}_{v}^{D R}=\widetilde{\mathcal{N}}_{v}+\frac{\mathcal{N}_{v}^{1}}{\epsilon} \tag{38}
\end{equation*}
$$

where, e.g., $\widetilde{\mathcal{M}}_{v}$ is the finite contribution obtained using the finite pieces of the scalar and tensor coefficient integrals including the finite contributions from rational terms arising in ultraviolet tensor coefficient integrals.

### 4.3 UNIVERSAL BUILDING BLOCKS

Based on the observation that the same one-loop virtual amplitudes appear in many processes (Fig. 6), we are aiming to collect a basis of universal building blocks, which can be used to compute all of the $2 \rightarrow 4$ processes at LHC at the QCD one-loop level (Similar to the philosophy of older versions of MADGRAPH [191] calling the HELAS [192] routines). This methodology of collecting topologies in groups has been proved very successful in the program VBFNLO, where for example a boxline routine, first line of Fig. 6, is computed and applied to $p p \rightarrow V V, p p \rightarrow V V V, p p \rightarrow V V j$ and EW production of $p p \rightarrow V j j$ and $p p \rightarrow H V j j$.


Fig. 6: Boxline contributions appearing in different processes.

To do that, we use the effective current approach described and applied in Refs. [39, 47, 31, 193, 21]. As illustration, the first diagram of the second raw of Fig. 6is used. This can be written as,

$$
\begin{equation*}
A_{V_{1} V_{2} V_{3} V_{4}, \tau}=J_{V_{1}^{*}}^{\mu_{1}} J_{V_{2}^{*}}^{\mu_{2}} \mathcal{M}_{\mu_{1} \mu_{2}, \tau} \equiv \mathcal{M}_{V_{1}^{*} V_{2}^{*}, \tau} \tag{39}
\end{equation*}
$$

where the color indices have been omitted. Here, $J_{V_{1}^{*}}^{\mu_{1}}$ and $J_{V_{2}^{*}}^{\mu_{2}}$ represent effective polarization vectors in the unitarity gauge for the EW sector including finite width effects in the scheme of Refs. [194, 195] and propagator factors, e.g.,

$$
\begin{equation*}
J_{V_{1}^{*}}^{\mu_{1}}\left(q_{1}\right)=\frac{-i}{q_{1}^{2}-M_{V_{1}^{*}}^{2}-i M_{V_{1}^{*}} \Gamma_{V_{1}^{*}}}\left(g_{\mu}^{\mu_{1}}-\frac{q_{1}^{\mu_{1}} q_{1 \mu}}{q_{1}^{2}-M_{V_{1}^{*}}^{2}-i M_{V_{1}^{*}} \Gamma_{V_{1}^{*}}}\right) \Gamma_{V_{1}^{*} V_{1} V_{3}}^{\mu} \tag{40}
\end{equation*}
$$

with $\Gamma_{V_{1}^{*}}$, the width of the $V_{1}^{*}$ vector boson, and $\Gamma_{V_{1}^{*} V_{1} V_{3}}^{\mu}$, the triple vertex, which can also contain the leptonic decay of the EW vector bosons including all off-shell effects or BSM physics. In this manner, we can then concentrate in computing, instead of $A_{V_{1} V_{2} V_{3} V_{4}, \tau}$, the virtual correction to two massive vector bosons attached to the quark line, $\mathcal{M}_{V_{1}^{*} V_{2}^{*}, \tau}$, or equivalently $\mathcal{M}_{\mu_{1} \mu_{2}, \tau}$, where the polarization vectors or effective currents have been factored out. In our approach, this basic building block is the so-called Boxline, which is computed only once and re-used in different processes.

We plan to do a classification of all the topologies that appear at 1 loop level for up to $2 \rightarrow 4$ processes and install a library with all the basic one-loop building blocks already computed and simplified. This would be an advantage since, for example for $q q \rightarrow V V V V$ production, up to 24 hexagons for a single subprocess would appear, corresponding to the permutations of the vector bosons on the hexagon of Eq. 34. In this approach, the amplitude is obtained by calling the same one-loop amplitude 24 times with the corresponding ordering of momenta and polarization vectors. We aim towards an automation of this procedure, which will result into a faster and shorter final FORTRAN code generation. The specific building blocks are collected into groups with specific gauge and IR factorization properties, e.g, factorization of the IR divergences against the corresponding born, known behavior under Ward identity checks.

In Fig. 7. we present the topologies that have been computed and tested. In the first line, corrections to a quark line with the emission of $\mathrm{V}_{n}$ vector bosons in a fixed order are represented for 4 different topologies. (The first 2 were explained in detail in Ref. [185], including their stability behavior). We have only depicted the virtual amplitude with the higher complexity for a giving building block, e.g. the boxline of Fig.6is obtained from the first diagram with two vector bosons attached, i.e., $n=2$ in $V_{n}$. The first two topologies of the second line are collected by putting together all possible Feynman-diagrams with a fixed order of the vector bosons and attaching it to the quark lines in all possible ways. The crossing of the fermion lines are treated as independent building blocks and are not depicted. Finally, the fermion-loop corrections for a fixed order of vector bosons, $V_{n}$, are computed in the last diagram of the second line

The use of modular structure routines, as the above presented, has been proved to be an advantage in the program VBFNLO [42, 41] since once a structure is computed and checked it can be re-used for different processes. For example, using the building blocks of the first and second topology together with the fermion-loop diagrams, results at NLO QCD for all $V V V$ [39, 47, 46, 45, 43, 44], several $V V j$ [31, 32, 196, 197], $H \gamma j j$ [198] and $W \gamma \gamma j$ [21] production channels have been computed recently. The last one representing the first calculation at this accuracy falling in the category of $V V V+j$ production. Up to the pentagon level, these building blocks are publicly available as part of the VBFNLO [42, 41] package together with the tensor reduction routines, excluding the routines for small Gram determinants which will become available in the future, in addition to the other building blocks.

### 4.4 CONCLUSIONS

A program which automatically evaluates one-loop amplitudes for up to $2 \rightarrow 4$ processes has been presented based on the traditional Feynman-diagram approach. The program has been developed in the framework of Mathematica and FeynCalc and writes down automatically the simplified expression to FORTRAN. Up to the pentagon level and for massless propagators, the code can be evaluated numerically inside Mathematica with unlimited precision which can be used for testing purposes. For the reduction of tensor integrals, we have developed a library that includes expansion for small Gram determinants. Using the leptonic tensor formalism, we are building a library of universal one-loop building blocks, which can be used to compute several processes at NLO QCD. Recently, following this strategy, we have reported results for all $V V V$ [39, 47, 46, 45, 43, 44], several $V V j$ [31, 32, 196, 197], $H \gamma j j$ [198] and $W \gamma \gamma j$ [21] production channels inside the VBFNLO collaboration. The ultimate goal is to generalize the library to compute all of the $2 \rightarrow 4$ processes at LHC at the QCD one-loop level, similar to the philosophy of older versions of MADGRAPH [191] calling the HELAS [192] routines,


Fig. 7: Topologies of universal building one-loop blocks. Only the most complicated diagram of each topology is depicted, e.g, the boxline of Fig 6 is obtained from the first diagram with two vector bosons attached, i.e., $V_{n}, n=2$.
and deliver a Mathematica package compatible with FeynArts [132], which can be used to compute full one-loop amplitudes automatically using the universal building blocks, resulting into a faster and shorter code generation.

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## 5. THE TWO-LOOP QCD VIRTUAL AMPLITUDE FOR W PAIR PRODUCTION WITH FULL MASS DEPENDENCE 7

### 5.1 INTRODUCTION

One of the main aims in the Large Hadron Collider (LHC) physics program is undoubtedly the discovery (or the exclusion) of the Higgs boson which is responsible for the fermion and gauge boson masses and also part of the mechanism of dynamical breaking of the Electroweak (EW) symmetry. Another important goal for the LHC is the precise measurement of the hadronic production of gauge boson pairs, $W W, W Z, Z Z, W \gamma, Z \gamma$, this in connection to the investigation of the non-Abelian gauge structure of the SM . W pair production,

$$
\begin{equation*}
q \bar{q} \rightarrow W^{+} W^{-}, \tag{41}
\end{equation*}
$$

[^121]plays an essential role as it serves as a signal process in the search for New Physics and also is the dominant irreducible background to the Higgs discovery channel $p p \rightarrow H \rightarrow W^{*} W^{*} \rightarrow l \bar{\nu} \bar{l}^{\prime} \nu^{\prime}$, in the intermediate Higgs mass range [199]. Both ATLAS and CMS collaborations have released first values for the $W W$ cross section [200, 201].

The process (41) is currently known at next-to-leading order (NLO) accuracy [202, 203, 204, 205, 206, 157, ?]. The NLO corrections were proven to be large enhancing the tree-level result by almost $70 \%$ which falls to a (still) large $30 \%$ after imposing a jet veto. Therefore, if a theoretical estimate for the W pair production is to be compared against experimental measurements at the LHC, one is bound to go one order higher in the perturbative expansion, namely, to the next-to-next-to-leading order (NNLO). This would allow, in principle, an accuracy of around $10 \%$.

High accuracy for the W pair production is also needed when the process is studied as background to Higgs production in order to match accuracies between signal and background. The signal process for the Higgs discovery via gluon fusion, $g g \rightarrow H$, as well as the process $H \rightarrow W W \rightarrow l \bar{\nu} \bar{l}^{\prime} \nu^{\prime}$ are known at NNLO [207, 208, 209, 210, 211, 212, 213, 214, 215, 216], whereas the EW corrections are known beyond NLO [217]. Another process that needs to be included in the background is the W pair production in the loop induced gluon fusion channel,

$$
\begin{equation*}
g g \rightarrow W^{+} W^{-} \tag{42}
\end{equation*}
$$

The latter contributes at $\mathcal{O}\left(\alpha_{s}^{2}\right)$ relative to the quark-anti-quark-annihilation channel but is nevertheless enhanced due to the large gluon flux at the LHC [218, 219].

The first main difficulty in studying the NNLO QCD corrections for W pair production is the calculation of the two-loop virtual amplitude since it is a $2 \rightarrow 2$ process with massive external particles. We have already computed the virtual corrections at the high energy limit [220, 97, 221]. However, this is not enough as it cannot cover the kinematical region close to threshold. Therefore, in order to cover all kinematical regions we proceed as follows. We perform a deep expansion in the W mass around the high energy limit which in combination with the method of numerical integration of differential equations [222, 223, 224] allows us the numerical computation of the two-loop amplitude with full mass dependence over the whole phase space.

### 5.2 THE HIGH ENERGY LIMIT

The methodology for obtaining the massive amplitude in the high energy limit, namely the limit where all the invariants are much larger than the W mass, is similar to the one followed in Refs. [225, 226]. The amplitude is reduced to an expression that only contains a small number of integrals (master integrals) with the help of the Laporta algorithm [227]. In the calculation for the two-loop amplitude there are 71 master integrals. Next step is the construction, in a fully automatised way, of the Mellin-Barnes (MB) representations [228, 229] of all the master integrals by using the MBrepresentation package [230]. The representations are then analytically continued in the number of space-time dimensions by means of the MB package [231], thus revealing the full singularity structure. An asymptotic expansion in the mass parameter ( W mass) is performed by closing contours and the integrals are finally resummed, either with the help of XSummer [232] or the PSLQ algorithm [233]. The result is expressed in terms of harmonic polylogarithms.

### 5.3 POWER CORRECTIONS AND NUMERICAL EVALUATION

The high energy limit by itself is not enough, as was mentioned before. The next step, following the methods applied in Ref. [234], is to compute power corrections in the W mass. Power corrections are good enough to cover most of the phase space, apart from the region near threshold as well as the regions corresponding to small angle scattering.

We recapitulate here some of the notation of Ref. [221] for completeness. The charged vectorboson production in the leading partonic scattering process corresponds to

$$
\begin{equation*}
q\left(p_{1}\right)+\bar{q}\left(p_{2}\right) \rightarrow W^{-}\left(p_{3}, m\right)+W^{+}\left(p_{4}, m\right) \tag{43}
\end{equation*}
$$

where $p_{i}$ denote the quark and W momenta and $m$ is the mass of the W boson.
We have chosen to express the amplitude in terms of the kinematic variables $x$ and $m_{s}$ which are defined to be

$$
\begin{equation*}
x=-\frac{t}{s}, \quad m_{s}=\frac{m^{2}}{s} \tag{44}
\end{equation*}
$$

where

$$
\begin{equation*}
s=\left(p_{1}+p_{2}\right)^{2} \text { and } t=\left(p_{1}-p_{3}\right)^{2}-m^{2} \tag{45}
\end{equation*}
$$

The variation then of $x$ within the range $[1 / 2(1-\beta), 1 / 2(1+\beta)]$, where $\beta=\sqrt{1-4 m^{2} / s}$ is the velocity, corresponds to angular variation between the forward and backward scattering.

It should be evident that any master integral $M_{i}$ can be written then as

$$
\begin{equation*}
M_{i}=M_{i}\left(m_{s}, x, \epsilon\right)=\sum_{j=k}^{l} \epsilon^{j} I_{i j}\left(m_{s}, x\right) \tag{46}
\end{equation*}
$$

where $\epsilon$ is the usual regulator in dimensional regularization $(d=4-2 \epsilon)$ and the lowest power of $\epsilon$ in the sum can be -4 .

The crucial point now is that the derivative of any Feynman integral with respect to any kinematical variable is again a Feynman integral with possibly higher powers of denominators or numerators which can also be reduced anew in terms of the initial set of master integrals. This means that one can construct a partially triangular system of differential equations in the mass, which can subsequently be solved in the form of a power series expansion, with the expansion parameter in our case being $m_{s}$ following the conventions above.

Let us differentiate with respect to $m_{s}$ and $x$, we will then have respectively

$$
\begin{equation*}
m_{s} \frac{d}{d m_{s}} M_{i}\left(m_{s}, x, \epsilon\right)=\sum_{j} C_{i j}\left(m_{s}, x, \epsilon\right) M_{j}\left(m_{s}, x, \epsilon\right) \tag{47}
\end{equation*}
$$

and

$$
\begin{equation*}
x \frac{d}{d x} M_{i}\left(m_{s}, x, \epsilon\right)=\sum_{j} C_{i j}^{\prime}\left(m_{s}, x, \epsilon\right) M_{j}\left(m_{s}, x, \epsilon\right) \tag{48}
\end{equation*}
$$

We use Eq. 47) to obtain the mass corrections for the master integrals calculating the power series expansion up to order $m_{s}^{11}$ (see also Ref. [234] for more details). This deep expansion in $m_{s}$ should be sufficient for most of the phase space but still not enough to cover the whole allowed kinematical region. The way to proceed from this point is to numerically integrate the system of differential equations.

In particular, we choose to work with the master integrals in the form of Eq. 46, where the $\epsilon$ dependence is explicit. We can then work with the coefficients of the $\epsilon$ terms and accordingly have

$$
\begin{equation*}
m_{s} \frac{d}{d m_{s}} I_{i}\left(m_{s}, x\right)=\sum_{j} J_{i j}^{M}\left(m_{s}, x\right) I_{j}\left(m_{s}, x\right) \tag{49}
\end{equation*}
$$

and

$$
\begin{equation*}
x \frac{d}{d x} I_{i}\left(m_{s}, x\right)=\sum_{j} J_{i j}^{X}\left(m_{s}, x\right) I_{j}\left(m_{s}, x\right) \tag{50}
\end{equation*}
$$

where the Jacobian matrices $J^{M}$ and $J^{X}$ have rational function elements.

By using this last system of differential equations, one can obtain a full numerical solution to the problem. What we are essentially dealing now with is an initial value problem and the main requirement is to have the initial conditions to proper accuracy. The initial conditions, namely the values of the master integrals at a proper kinematical point which we call initial point, are provided by the power series expansion. The initial point has to be chosen somewhere in the high energy limit region, where $m_{s}$ is small and therefore, the values obtained by the power series are very accurate. Starting from there, one can evolve to any other point of the phase space by numerically integrating the system of differential equations Eq. (49) and Eq. (50).

We parametrise with a suitable grid of points the region close to threshold and then we calculate the master integrals for all points of the grid by evolving as described previously. Given that the master integrals have to be very smooth (we remain above all thresholds) one can use, after having the values for the grid points, interpolation to get the values at any point of the region. We use 1600 points for the grid and take as initial conditions the values of the master integrals at the point $m_{s}=5 \times 10^{-3}, x=1 / 4$. The relative errors at that point were estimated not to exceed $10^{-18}$.

The numerical integration is performed by using one of the most advanced software packages implementing the variable coefficient multistep method (ODEPACK) [235]. We use quadruple precision to maximise accuracy. The values at any single grid point can be obtained in about 15 minutes in average (with a typical 2 GHz Intel Core 2 Duo system) after compilation with the Intel Fortran compiler. The accuracy is around 10 digits for most of the points of the grid. It is also worth noting that in order to perform the numerical integration one needs to deform the contour in the complex plane away from the real axis. This is due to the fact that along the real axis there are spurious singularities. We use an elliptic contour and we achieve a better estimate of the final global error by calculating more than once for each point of the grid, using each time different eccentricities. Grids of solutions can actually be constructed, which will be subsequently interpolated when implemented as part of a Monte Carlo program.

One very stringent test we use to cross-check the correctness and also the accuracy of our calculation is to compare the infrared pole structure of our two-loop result against the one predicted by Catani [182] (see also Refs. [236, 237, 238]). According to Catani, the infrared poles of the interference of the tree and the two-loop amplitudes follow a generic formula which in our case, since we work with the rescaled variables $m_{s}$ and $x$, can be cast into the following form:

$$
\begin{equation*}
\mathcal{C}_{\text {atani }}^{(0 \times 2)}\left(m_{s}, x, \frac{s}{\mu}\right)=2 \operatorname{Re}\left\{\mathrm{I}^{(1)}(\mathrm{ffl})\left\langle\mathrm{M}^{(0)} \mid \mathrm{M}^{(1)}\right\rangle+\mathrm{I}^{(2)}(\mathrm{ff})\left\langle\mathrm{M}^{(0)} \mid \mathrm{M}^{(0)}\right\rangle\right\} \tag{51}
\end{equation*}
$$

where $\mathrm{M}^{(0)}$ and $\mathrm{M}^{(1)}$ are the tree level and one-loop amplitudes respectively and $\mu$ is the renormalization scale. The operators $\mathrm{I}^{(1)}(\mathrm{ffl})$ and $\mathrm{I}^{(2)}(\mathrm{ffl})$ encode the information for the infrared pole structure and their exact expressions can be found in Ref. [97].

The way to perform the test is straightforward. For each point of the grid with coordinates $\left(m_{s(i)}, x_{(i)}\right)$, we compute the numerical value of the two-loop amplitude $\left(\mathrm{M}^{(2)}\right)$ interfered with the tree level amplitude

$$
\begin{equation*}
\mathcal{A}^{(0 \times 2)}\left(m_{s(i)}, x_{i}, \frac{s}{\mu}\right)=\left\langle\mathrm{M}^{(0)} \mid \mathrm{M}^{(2)}\right\rangle+\left\langle\mathrm{M}^{(2)} \mid \mathrm{M}^{(0)}\right\rangle \tag{52}
\end{equation*}
$$

by numerically integrating the differential equations as described previously and we also calculate the numerical value of the quantity $\mathcal{C}_{\text {atani }}^{(0 \times 2)}\left(m_{s(i)}, x_{(i)}, \frac{s}{\mu}\right)$ by using Eq. 51). Then, all we need to make sure is that the infrared singularities of the quantity $\left\{\mathcal{A}^{(0 \times 2)}\left(m_{s(i)}, x_{i}, \frac{s}{\mu}\right)-\mathcal{C}_{\text {atani }}^{(0 \times 2)}\left(m_{s(i)}, x_{i}, \frac{s}{\mu}\right)\right\}$ cancel numerically for every point $\left(m_{s(i)}, x_{(i)}\right)$ of the grid (ultraviolet divergencies have been removed by renormalization). We will not present here any numbers since the aim was to describe the general methods. The details and the results of the study will be presented in a future publication [239].

### 5.4 CONCLUSIONS

W pair production via quark-anti-quark-annihilation is an important signal process in the search for New Physics as well as the dominant irreducible background for one of the main Higgs discovery channels: $H \rightarrow W W \rightarrow 4$ leptons. Therefore, the accurate knowledge of this process is essential for the LHC. After having calculated the two-loop and the one-loop-squared virtual QCD corrections to the W boson pair production in the high energy limit we proceed to the next step. Namely, we use a combination of a deep expansion in the W mass around the high energy limit and of numerical integration of differential equations to compute the two-loop amplitude with full mass dependence over the whole phase space. A strigent cross-check of our calculation is to verify that the infrared structure of our result agrees with the prediction of the Catani formalism for the infrared structure of QCD amplitudes.

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## 6. COMPUTATION OF INTEGRATED SUBTRACTION TERMS NUMERICALLY ${ }^{8}$


#### Abstract

We report on a numerical representation of the integrated subtraction terms of the NNLO subtraction scheme defined in Refs. [240, 241, 242, 243]. The integrated approximate cross sections themselves can be written as products of insertion operators (in colour space) times the Born, or the one-loop cross section. The insertion operator is constructed from the numerical representation of the integrated subtraction terms. We give selected results for the integrated doubly-collinear subtraction term.


### 6.1 INTRODUCTION

We consider the NNLO correction to a generic $m$-jet observable,

$$
\begin{equation*}
\sigma^{\mathrm{NNLO}}=\int_{m+2} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}} J_{m+2}+\int_{m+1} \mathrm{~d} \sigma_{m+1}^{\mathrm{RV}} J_{m+1}+\int_{m} \mathrm{~d} \sigma_{m}^{\mathrm{VV}} J_{m} . \tag{53}
\end{equation*}
$$

The three contributions on the right hand side are separately divergent in $d=4$ dimensions, but their sum is finite for IR safe observables. To obtain the finite NNLO correction, we first continue analytically all integrals to $d=4-2 \epsilon$ dimensions and then rewrite Eqn. (53) as

$$
\begin{equation*}
\sigma^{\mathrm{NNLO}}=\int_{m+2} \mathrm{~d} \sigma_{m+2}^{\mathrm{NNLO}}+\int_{m+1} \mathrm{~d} \sigma_{m+1}^{\mathrm{NNLO}}+\int_{m} \mathrm{~d} \sigma_{m}^{\mathrm{NNLO}} \tag{54}
\end{equation*}
$$

that is a sum of three integrals where the integrands,

$$
\begin{gather*}
\mathrm{d} \sigma_{m+2}^{\mathrm{NNLO}}=\left\{\mathrm{d} \sigma_{m+2}^{\mathrm{RR}} J_{m+2}-\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{2}} J_{m}-\left[\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}} J_{m+1}-\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{12}} J_{m}\right]\right\}_{\epsilon=0},  \tag{55}\\
\mathrm{~d} \sigma_{m+1}^{\mathrm{NNLO}}=\left\{\left[\mathrm{d} \sigma_{m+1}^{\mathrm{RV}}+\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}}\right] J_{m+1}-\left[\mathrm{d} \sigma_{m+1}^{\mathrm{RV}, \mathrm{~A}_{1}}+\left(\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}}\right)^{\mathrm{A}_{1}}\right] J_{m}\right\}_{\epsilon=0}, \tag{56}
\end{gather*}
$$

and

$$
\begin{equation*}
\mathrm{d} \sigma_{m}^{\mathrm{NNLO}}=\left\{\mathrm{d} \sigma_{m}^{\mathrm{VV}}+\int_{2}\left[\mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{2}}-\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{12}}\right]+\int_{1}\left[\mathrm{~d} \sigma_{m+1}^{\mathrm{RV}, \mathrm{~A}_{1}}+\left(\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}}\right)^{\mathrm{A}_{1}}\right]\right\}_{\epsilon=0} J_{m}, \tag{57}
\end{equation*}
$$

[^122]are integrable in four dimensions by construction. The approximate cross sections $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{2}}$ and $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}$ regularise the doubly- and singly-unresolved limits of the real-emission contribution, $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}}$ respectively. The double subtraction due to the overlap of these two terms is compensated by $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{12}}$. These terms are given explicitly in Ref. [242]. Finally, $\mathrm{d} \sigma_{m+1}^{\mathrm{RV}, \mathrm{A}_{1}}$ and $\left(\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}\right)^{\mathrm{A}_{1}}$ regularise the singly-unresolved limits of $\mathrm{d} \sigma_{m+1}^{\mathrm{RV}}$ and $\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}$ respectively. They are given explicitly in Ref. [243].

The construction of each approximate cross section in Eqns. (55-57) is based on the known and universal IR limits of tree level and one-loop squared matrix elements, and proceeds in two steps. First, the IR factorisation formulae are written in such a way that their complicated overlap structure can be disentangled ("matching of limits") [240, 244]. Second, we define "extensions" of the formulae, so that they are unambiguously defined away from the strict IR limits [241, 242, 243]. These extensions are defined by the use of various momentum mappings that map a set of $m+1$ or $m+2$ momenta into a set of $m$ momenta,

$$
\begin{equation*}
\{p\}_{m+1} \longrightarrow\{\tilde{p}\}_{m} \quad \text { and } \quad\{p\}_{m+2} \longrightarrow\{\tilde{p}\}_{m} \tag{58}
\end{equation*}
$$

such that (i) the delicate structure of cancellations among the matched limit formulae in various limits is respected (ii) exact momentum conservation is implemented, and (iii) the original $m+1$ or $m+2$ particle phase space factorises exactly into the product of an $m$ particle phase space and a one- or two-particle phase space measure,

$$
\begin{equation*}
\mathrm{d} \phi_{m+r}\left(\{p\}_{m+r} ; Q\right)=\mathrm{d} \phi_{m}\left(\{\tilde{p}\}_{m} ; Q\right)\left[\mathrm{d} p_{r, m}\right], \quad r=1,2 . \tag{59}
\end{equation*}
$$

To finish the definition of the scheme, one must compute once and for all the one- and two-particle integrals, denoted formally as $\int_{1}$ and $\int_{2}$, appearing in Eqns. 5657 .

In general the integrated subtraction terms are integrals of extensions over the whole phase space of combinations of the QCD splitting functions and squared soft currents. In this proceedings we discuss two examples: (i) the singly-collinear subtractions $\mathcal{C}_{i r}^{(\ell, 0)}$ and (ii) the doubly-collinear subtractions $\mathcal{C}_{i r, j s}^{(0,0)}$, which are part of $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}$ and $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{2}}$ in Eqn. 55 , respectively. The precise definitions of these terms can be found in Ref. [242]. The meaning of the superscript is irrelevant for our present purpose (also explained in Ref. [242]).

Denoting a generic subtraction term by $\mathcal{X}^{(\ell, k)}$ (such as $\mathcal{C}_{i r}^{(\ell, 0)}$ ) the integrated counterterms can be written in the following general form:

$$
\begin{equation*}
\int_{r} \mathcal{X}^{(\ell, k)}=\left[\frac{\alpha_{\mathrm{s}}}{2 \pi} S_{\epsilon}\left(\frac{\mu^{2}}{Q^{2}}\right)^{\epsilon}\right]^{r+\ell} N_{X}(\epsilon) X^{(\ell)}(x, \ldots) \operatorname{Re}\left\langle\mathcal{M}_{m}^{(0)}(\{\tilde{p}\})\right| \boldsymbol{T}_{i} \cdot \boldsymbol{T}_{j} \ldots\left|\mathcal{M}_{m}^{(k)}(\{\tilde{p}\})\right\rangle, \tag{60}
\end{equation*}
$$

where $S_{\epsilon}=(4 \pi)^{\epsilon} / \Gamma(1-\epsilon)$, and $X^{(\ell)}(x, \ldots)$ represents a function that depends on kinematical invariants of the factorized $m$-parton phase space. It results in the integration of the subtraction term $\mathcal{X}^{(\ell, k)}$ over the factorized phase spaces [ $\mathrm{d} p_{r, m}$ ] in Eqn. 59). In a NNLO computation the possible cases are $r+\ell+k=1$ with $\ell+k=0$ or 1 , and $r=2$ with $\ell+k=0$. We use the colour- and spin-state notation of Ref. [236], when the amplitude for a scattering process involving $m$ final-state momenta, $\left|\mathcal{M}_{m}^{(k)}\right\rangle$, is an abstract vector in colour and spin space; $k$ denotes the number of loops. Colour interactions at QCD vertices are represented by associating colour charges $\boldsymbol{T}_{i}$ with the emission of a gluon from each parton $i$. There are $2 r$ such colour charges. Then the functions $X^{(\ell)}$ are dimensionless in colour-space. For certain subtraction terms, universal, possibly $\epsilon$-dependent numerical factors, $N_{X}(\epsilon)$ appear naturally, which can be factored out. Our purpose is to compute all functions $X^{(\ell)}$, which we discuss next.

### 6.2 INTEGRATING THE COUNTERTERMS

The actual computation of the integrated counterterms leads to a large number of multi-dimensional integrals. The ultimate goal is to find the analytical form of the coefficients of a Laurent expansion (in
$\epsilon$ ) of these integrals, which turns out to be a rather tedious job. In order to compute these coefficients as efficiently as possible, we have explored several methods.

First, it is possible to extend the method of integration-by-parts identities and solving of differential equations, developed for computing multi-loop Feynman integrals [245, 246], to the relevant phase space integrations [247]. This method yields $\epsilon$-expansions with fully analytical coefficients, with the final results being expressed in terms of two-dimensional harmonic polylogarithms (after a suitable basis extension, see Ref. [247] for details). This approach was used successfully to compute a class of singlyunresolved integrals [247].

Second, the phase space integrals that arise can be computed via the method of Mellin-Barnes (MB) representations [228, 229, 248]. Here we obtain the $\epsilon$-expansion coefficients in terms of complex contour integrals over $\Gamma$-functions. Performing these integrals by the use of the residue theorem, a representation in terms of harmonic sums is obtained. In many cases, the sums can be evaluated in a closed form, yielding an analytical result. In some instances however, we find multi-dimensional MB integrals that are very difficult to compute fully analytically. Nevertheless, in these situations a direct numerical evaluation of the appropriate MB representations provides a fast and reliable way to obtain final results with small numerical uncertainties. We stress that for phenomenological applications, this is all that is required, since the numerical uncertainty of the complete computation is dominated by the phase space integrations. We have used the MB method to compute all singly-unresolved integrals [249], and all two-particle integrals appearing in $\int_{2} \mathrm{~d} \sigma_{m+2}^{R R, A_{12}}$ as well [91].

Finally, the method of iterated sector decomposition [250] can also be used to calculate the integrals we encounter [251]. Sector decomposition produces a representation of the $\epsilon$-expansion where the coefficients are given in terms of (mostly quite cumbersome) finite integrals over the unit hypercube. The analytical evaluation of these integrals is not feasible except for the simplest cases. Nevertheless, this method is simple to implement and can be automated to a large extent. In fact there are several computer programs that use various implementations of sector decomposition to provide numerical values of coefficients of the powers of $\epsilon$ in the Laurent expansion of dimensionally regulated integrals [252, 253, 254]. We found the program $\operatorname{SecDec}$ powerful and flexible to generate sufficiently precise values of our integrated subtraction terms.

Choosing the Cuhre integrator implemented in SecDec, we can easily reach $10^{-7}$ relative precision for the integration. Such precision is sufficient for our purposes: (i) to demonstrate the cancellation of the $\epsilon$ poles numerically, and (ii) to compute the finite integrals in Eqns. (56) and (57). As the numerical uncertainty of the second item is limited more by the Monte Carlo integration over the $m+1$ and $m$ particle phase spaces, for item (ii) much lower (not better than $10^{-3}$ ) precision is sufficient. This looser requirement on the precision for the $\mathrm{O}(1)$ terms and the fact that the integrated subtraction terms are smooth functions of their parameters, with logarithmic behaviour for asymptotically small values of the parameters, makes possible that we find sufficient approximations to the integrated subtraction terms.

### 6.3 APPROXIMATE INTEGRATED SUBTRACTION TERMS

The computation of the integrated subtraction terms at any given values of the kinematical parameters, as required in the Monte Carlo integration over the phase space, is not feasible. In order to demonstrate the cancellation of the $\epsilon$ poles numerically we can choose several randomly selected phase space points and evaluate the necessary integrals with high precision. The cancellation cannot depend on the particular phase space point. In the case of the finite remainders, in order to compute the phase space integrals in Eqns. 56 ) and (57), we are able to find sufficiently precise approximations to the integrated subtraction terms using a procedure that can be automated to high degree. The latter point is also important as there are several hundred integrals to compute. In the following, we outline our procedure for two cases: (i) an example with integrals depending on one kinematical parameter, $\left(\int_{1} \mathcal{X}^{(\ell, k)}=\int_{1} \mathcal{C}_{i r}^{(\ell, 0)}\right)$ and (ii) another example with integrals depending on two kinematical parameters, $\left(\int_{2} \mathcal{X}^{(\ell, k)}=\int_{2} \mathcal{C}_{i r, j s}^{(0,0)}\right)$.

In order to compute $\int_{1} \mathcal{C}_{i r}^{(\ell, 0)}$, we have to integrate the azimuthally averaged Altarelli-Parisi splitting functions $P_{f_{i} f_{r}}^{(\ell)}\left(z_{i, r}, z_{r, i} ; \epsilon\right)$ in $4-2 \epsilon$ dimensions for the splitting process $f_{i r} \rightarrow f_{i}+f_{r}$, with $z_{i}$ being the momentum fraction of parton $f_{i}$. It was discussed in Ref. [249] that the corresponding functions $C_{i r}^{(\ell)}$ can be expressed as combinations of the integrals (we changed the notation from $\mathcal{I}$ to $\mathcal{I}_{C}$ )

$$
\begin{equation*}
\mathcal{I}_{C}\left(x ; \epsilon, \alpha_{0}, d_{0}, \kappa, k, \delta, g_{I}^{( \pm)}\right)=\frac{16 \pi^{2}}{S_{\epsilon}} Q^{2 \epsilon} \int_{1}\left[\mathrm{~d} p_{1, m+1}^{(i r)}\right] \frac{z_{r}^{k+\delta \epsilon}}{s_{i r}^{1+\kappa \epsilon}} g_{I}^{( \pm)}\left(z_{r}\right) f\left(\alpha_{0}, \alpha_{i r}, d(m, \epsilon)\right) . \tag{61}
\end{equation*}
$$

In terms of explicit integration variables these collinear integrals have the general form [249]

$$
\begin{align*}
& \mathcal{I}_{C}\left(x ; \epsilon, \alpha_{0}, d_{0} ; \kappa, k, \delta, g_{I}^{( \pm)}\right)=x \int_{0}^{\alpha_{0}} \mathrm{~d} \alpha \alpha^{-1-(1+\kappa) \epsilon}(1-\alpha)^{2 d_{0}-1}[\alpha+(1-\alpha) x]^{-1-(1+\kappa) \epsilon} \\
& \quad \times \int_{0}^{1} \mathrm{~d} v[v(1-v)]^{-\epsilon}\left(\frac{\alpha+(1-\alpha) x v}{2 \alpha+(1-\alpha) x}\right)^{k+\delta \epsilon} g_{I}^{( \pm)}\left(\frac{\alpha+(1-\alpha) x v}{2 \alpha+(1-\alpha) x}\right) . \tag{62}
\end{align*}
$$

The necessary functions $g_{I}^{( \pm)}$are listed in Ref. [249], where analytic results of these integrals for $\alpha_{0}=1$ and $d_{0}=3$ are also presented.

Our present goal is to provide sufficiently precise numerical approximations to the functions $\mathcal{I}_{C}(x)$ in a simple way. The motivation is that often it is difficult to perform the analytic computation with arbitrary values of the parameters. For instance, the derivation with $\alpha_{0}=1$ is rather different from a derivation with $\alpha_{0}<1$. Also, the choice for $d_{0}$ is to some extent arbitrary, and a new choice requires a completely new analytic computation. Thus, for the sake of flexibility we propose a fully numerical approach here.

First we used the program SecDec, modified such that it can compute the value of the integral at multiple values of the parameter $x$ in a single run. For simplicity, we call the $\mathrm{O}(1)$ terms of the integral 'measurements'. Then, inspired by the analytic results in Ref. [249], we fitted these measurements by combinations of logarithms and polynomials in $x$ of the form

$$
\begin{equation*}
\mathcal{F}_{C}\left(x ; \kappa=0, k, \delta=0, g_{I}^{( \pm)}=1\right)=\sum_{n=0}^{n_{\max }} P_{n}^{(m)}(x, k) \log ^{n}(x), \quad P_{n}^{(m)}(x, k)=\sum_{n=0}^{m} a_{n}^{(k)} x^{n} \tag{63}
\end{equation*}
$$

where the upper limit $n_{\max }$ is determined by the power $-n_{\text {max }}$ of the leading pole in the Laurentexpansion (in $\epsilon$ ) of the integral. As for the degree of the polynomials we tried several simple choices ( $m=1,2,3$ ). We found that splitting the region of the parameter space into an asymptotic ( $0<x \leq$ $10^{-4}$ ) and a non-asymptotic ( $10^{-4}<x \leq 1$ ) region, we could provide a fit with $m=2$ that approximates the analytic result within relative difference few times $10^{-4}$. The loss of relative precision is associated with phase space points where the function changes sign, and its numerical value is close to zero (around $x=0.2$ ).

In Fig. 8 we show the approximate function $\mathcal{F}_{C}\left(x ; \alpha_{0}, d_{0}, 0,-1,0,1\right)$ together with the 'measurements', which coincide with the known exact analytic result to at least six digit accuracy. We find very good agreement, which is characterized by the ratio of the two values in the lower panels. In Fig. 8 b we show the approximate function for $\alpha_{0}=0.1$ and $d_{0}=3-3 \epsilon$ together with the corresponding 'measurements'. In this case the analytic results are not available.

Building on the experience gained in studying the one-parameter case, we worked out a similar strategy for the integrated subtraction term $\int_{2} \mathcal{C}_{i r, j s}^{(0,0)}$. The corresponding functions $C_{i r, j s}^{(0,0)}$ can be ex-


Fig. 8: The fitted function $\mathcal{F}_{C}(x ; 0,-1,0,1)$ compared to the integral $\mathcal{I}(x ; 0,-1,0,1)$ at a) $\alpha_{0}=1$ and $d_{0}=3$, b) $\alpha_{0}=0.1$ and $d_{0}=3-3 \epsilon$.
pressed as combination of the integrals

$$
\begin{align*}
& \mathcal{I}_{2 C}\left(x_{i}, x_{j} ; \epsilon, \alpha_{0}, d_{0} ; k, l\right)=x_{i} x_{j} \int_{0}^{1} \mathrm{~d} \alpha \int_{0}^{1} \mathrm{~d} \beta \Theta\left(\alpha_{0}-\alpha-\beta\right) \\
& \quad \times(1-\alpha-\beta)^{2 d_{0}-2(1-\epsilon)} \alpha^{-1-\epsilon} \beta^{-1-\epsilon}\left(\alpha+(1-\alpha-\beta) x_{i}\right)^{-1-\epsilon}\left(\beta+(1-\alpha-\beta) x_{j}\right)^{-1-\epsilon} \\
& \quad \times \int_{0}^{1} \mathrm{~d} v v^{-\epsilon}(1-v)^{-\epsilon} \int_{0}^{1} \mathrm{~d} u u^{-\epsilon}(1-u)^{-\epsilon}\left(\frac{\alpha+(1-\alpha-\beta) x_{i} v}{2 \alpha+(1-\alpha-\beta) x_{i}}\right)^{k}\left(\frac{\beta+(1-\alpha-\beta) x_{j} u}{2 \beta+(1-\alpha-\beta) x_{j}}\right)^{l} . \tag{64}
\end{align*}
$$

We again run SecDec with $\alpha_{0}=0.1$ and $d_{0}=3-3 \epsilon$ at several hundred different values of the kinematic parameters to obtain the 'measurements'. To reach $10^{-7}$ relative precision for all such 'measurements' takes several hours on a single CPU. Then we fitted these 'measurements' with the function

$$
\begin{equation*}
\mathcal{F}_{2 C}\left(x_{i}, x_{j} ; k, l\right)=\sum_{n_{i}=0}^{n_{\max }} \sum_{n_{j}=0}^{n_{\max }-n_{i}} P_{n_{i}}^{(m)}\left(x_{i}, k, l\right) P_{n_{j}}^{(m)}\left(x_{j}, k, l\right) \log ^{n_{i}}\left(x_{i}\right) \log ^{n_{j}}\left(x_{j}\right) . \tag{65}
\end{equation*}
$$

We divide the parameter space $0<x_{i}, x_{j} \leq 1$ into four regions: (i) $0<x_{i}, x_{j} \leq 10^{-4}$, (ii) $0<x_{i} \leq$ $10^{-2}$ and $10^{-4}<x_{j} \leq 1$, (iii) $0<x_{j} \leq 10^{-2}$ and $10^{-4}<x_{i} \leq 1$, (iv) $10^{-2}<x_{i}, x_{j} \leq 1$. Using $m=2$, we are able to fit the original function $\mathcal{I}_{2 C}$ to per mille precision almost everywhere. The ratio of the fitted function $\mathcal{F}_{2 C}$ to the numerical evaluation of $\mathcal{I}_{2 C}$ is shown in Fig. 9 together whith the fitted function $\mathcal{F}_{2 C}$ itself.

## CONCLUSIONS

We have worked out a numerical procedure for providing simple approximations of the integrated subtraction terms of the NNLO subtraction scheme defined in Refs. [240, 241, 242, 243]. We use the publicly available program SecDec to compute the coefficients of the Laurent expansion of the necessary integrals to high numerical precision. We found that the integrals that depend on one or two kinematical invariants can be approximated with simple combinations of polynomials and logarithms. The precision of these approximations is usually at per mille or better.


Fig. 9: The ratio of the fitted function $\mathcal{F}_{2 C}\left(x_{i}, x_{j} ;-1, l\right)$ to the integral $\mathcal{I}_{2 C}\left(x_{i}, x_{j} ;-1, l\right)$. a) $\left.l=-1 \mathbf{b}\right)$ $l=0$ Also shown the fitted function $\mathcal{F}_{2 C}\left(x_{i}, x_{j} ;-1,-l\right)$.

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## Part III

## PARTON DISTRIBUTION FUNCTIONS

## 7. WHICH EXPERIMENTS CONSTRAIN THE GLUON PDF IN A GLOBAL QCD FIT? 9


#### Abstract

Based on computation of PDF-induced correlations, we identify the experiments in CTEQ and MSTW global QCD analyses that are sensitive to the gluon parton density in the proton. The Tevatron inclusive jet production at large momentum fractions $x$ and DIS charm quark production at moderately small $x$ show the strongest correlation with the gluon PDF. The strength of the PDF-induced correlation between the gluon PDF and inclusive (di)jet production data is different in the CTEQ and MSTW analyses.


### 7.1 Introduction

The parton distribution function (PDF) of gluons in a proton, $g(x, \mu)$, plays an important role in hadron collider phenomenology. It arises in cross sections for production of hadronic final states, massive scalar

[^123]

Fig. 10: CT10 and CTEQ 6.6 PDF uncertainty bands at $\mu=2 \mathrm{GeV}$ (left) and 100 GeV (right), taken from Ref. [255]. The CTEQ 6.6 best-fit PDFs and uncertainties are indicated by solid curves and hatched bands, while those of CT10 are indicated by dashed curves and dotted bands.
bosons, and hypothetical elementary particles, often in a combination with an overall normalization prefactor proportional to $\alpha_{s}$. The gluon distributions from CT10 [255] and CTEQ 6.6 [256] PDF sets are shown in Fig 10. The figure shows that the gluon PDF is constrained well by fitted experiments at the intermediate momentum fractions $x$, but the uncertainty grows in the region $x>0.1$. We may ask which experiments in the global fit impose the most significant constraints on the the gluon PDF. It is often said that the precise neutral-current DIS data provides the tightest constraints on the gluon PDF at $x$ of order $10^{-3}$, while inclusive jet production at the Tevatron plays the key role in constraining the gluon at $x>0.1$. However, the net PDF uncertainty reflects subtle interplay of numerous constraints imposed by QCD theory and multiple experiments, as well as various correlated uncertainties in experimental measurements. In this contribution, we identify the experiments with the strongest sensitivity to the gluon PDF by using a method of PDF-induced correlations that was developed in Refs. [256, 257, 258]. The analysis of correlations provides a systematic way to identify such experiments and also to establish specific ranges of $x$ and $Q$ where the correlations of the experimental data sets with the gluon PDF are the most pronounced.

### 7.2 Log-likelihood $\chi^{2}$ and PDF-induced correlations

The quality of theory description of an experimental data set can be quantified by the log-likelihood function $\chi^{2}$. Many high-energy physics experiments publish three kinds of measurement errors for each data point $i$ : the statistical error $\sigma_{i}$, uncorrelated systematic error $u_{i}$, and correlated systematic errors $\left\{\beta_{1 i}, \beta_{2 i}, \beta_{3 i} \ldots . \beta_{K i}\right\}$ of $K$ different types. To compare a theory prediction $T_{i}$ to the data value $D_{i}$ for a data point $i$, while accounting for all types of errors, the $\chi^{2}$ function can be constructed as [259, 260]

$$
\begin{equation*}
\chi^{2}=\sum_{\text {expt. }}\left[\sum_{i=1}^{N_{e}}\left(\frac{D_{i}-T_{i}(a)-\sum_{k=1}^{K} r_{k} \beta_{k i}}{\alpha_{i}^{2}}\right)^{2}+\sum_{k=1}^{K} r_{k}^{2}\right] \tag{66}
\end{equation*}
$$

where $\alpha_{i}^{2}=\sigma_{i}^{2}+u_{i}^{2}$ is the combined uncorrelated error; $r_{k}$ are random parameters describing each of $K$ correlated errors (each distributed according to the standard normal distribution); $N_{e}$ is the number of
the data points; and $K$ is the number of the sources of the correlated systematic errors.
Analytic minimization of the function (66) with respect to the correlated systematic parameters $r_{k}$ renders the following result [257, 259]:

$$
\begin{equation*}
\left.r_{k}\right|_{\text {best fit }}=\sum_{k^{\prime}=1}^{K} A_{k k^{\prime}}^{-1} B_{k^{\prime}}, \tag{67}
\end{equation*}
$$

where $A_{k k^{\prime}}$ and $B_{k}$ are given by

$$
\begin{equation*}
A_{k k^{\prime}}=\delta_{k k^{\prime}}+\sum_{i=1}^{N_{e}} \frac{\beta_{k i} \beta_{k^{\prime} i}}{\alpha_{i}^{2}}, \quad \text { and } \quad B_{k}=\sum_{i=1}^{N_{e}} \frac{\beta_{k i}\left(D_{i}-T_{i}\right)}{\alpha_{i}^{2}} . \tag{68}
\end{equation*}
$$

Substituting Eq. 67] into Eq. (66], we obtain a reduced $\chi^{2}$ function [257, 259],

$$
\begin{equation*}
\chi^{2}=\sum_{\text {expt. }}\left[\sum_{i=1}^{N_{e}} \frac{\left(D_{i}-T_{i}\right)^{2}}{\alpha_{i}^{2}}-\sum_{k, k^{\prime}=1}^{K} B_{k} A_{k k^{\prime}}^{-1} B_{k^{\prime}}\right] . \tag{69}
\end{equation*}
$$

In this function, the information about the systematic shifts in $r_{k}$ is included implicitly. Often, the influence of the correlated shifts on the PDFs is substantial.

Next, we wish to discuss correlations between PDF uncertainties of two variables, $X(\vec{a})$ and $Y(\vec{a})$, where $\vec{a}=\left\{a_{1}, a_{2}, \ldots, a_{N}\right\}$ is the vector of $N$ PDF parameters. The correlations can be computed either in the Hessian [256, 257, 258] or Monte-Carlo [261] approaches. In this note we will adopt the Hessian approach.

A symmetric PDF uncertainty $\Delta X$ corresponds to the maximal variation of $X$ for all combinations of PDF parameters that lie within the tolerance hypersphere $\Delta \chi^{2} \leq T^{2}$. This uncertainty is given by

$$
\begin{equation*}
\Delta X=\frac{1}{2} \sqrt{\sum_{i=1}^{N}\left[X_{i}^{+}-X_{i}^{-}\right]^{2}} \tag{70}
\end{equation*}
$$

in terms of the value $X_{0}$ of $X$ obtained with the central PDF set, and values $X_{i}^{+}$and $X_{i}^{-}$of $X$ obtained for maximal positive and negative displacements of each orthonormal PDF parameter $a_{i}$ within the tolerance hypersphere. The same "master equation" defines $\Delta Y$, the PDF uncertainty of the variable $Y$.

In the linear approximation, the pairs of values of $X$ and $Y$ that are allowed within the PDF uncertainty correspond to the points inside an ellipse in the $X-Y$ plane. The boundary of the ellipse is parametrically described by

$$
\begin{align*}
& X=X_{0}+\Delta X \cos \theta  \tag{71}\\
& Y=Y_{0}+\Delta Y \cos (\theta+\varphi) \tag{72}
\end{align*}
$$

where the parameter $\theta$ varies between 0 and $2 \pi$, and the relative phase angle $\varphi$ is a function of $X_{i}^{ \pm}$and $Y_{i}^{ \pm}$. The PDF uncertainties $\Delta X$ and $\Delta Y$ are calculated according to Eq. 70). The angle $\varphi$ is included between the gradients $\vec{\nabla} X$ and $\vec{\nabla} Y$ of $X$ and $Y$ in the PDF parameter space. Its cosine,

$$
\begin{equation*}
\cos \varphi=\frac{\vec{\nabla} X \cdot \vec{\nabla} Y}{\Delta X \Delta Y}=\frac{1}{4 \Delta X \Delta Y} \sum_{i=1}^{N}\left(X_{i}^{(+)}-X_{i}^{(-)}\right)\left(Y_{i}^{(+)}-Y_{i}^{(-)}\right) \tag{73}
\end{equation*}
$$

quantifies the degree of similarity in the PDF dependence of $X$ and $Y$. If $X$ and $Y$ are strongly correlated (corresponding to $\cos \varphi \rightarrow 1$ ) or anti-correlated $(\cos \varphi \rightarrow-1)$, the PDF uncertainties of $X$ and $Y$ are driven by essentially the same combinations of PDF parameters. Conversely, the PDF dependence of $X$ is independent from the PDF dependence of $Y$ if $\cos \varphi \approx 0$.

### 7.3 Which experiments are sensitive to the gluon PDF?

If an experimental cross section $\sigma$ strongly constrains a PDF $f_{a}(x, Q)$ for some combination of $x$ and $Q$, we expect that Eq. $\sqrt{73} \mid$ returns $|\cos \varphi|$ close to unity when using $X=f_{a / A}(x, Q)$ and $Y=\sigma$. If the experimental data set includes several data points, we can use $Y=\chi^{2}$. The strength of the constraint on the PDF from this experiment is determined by $|\cos \varphi|$ and the magnitude of $\chi^{2}$. In the majority of the fitted experiments, $\chi^{2} / N_{e}$ is close to 1 , so that $|\cos \varphi|$ tends to be more important for distinguishing between the sensitivities of the experiments than the magnitude of $\chi^{2}$.

Following this approach, we compute $\cos \varphi$ between the NLO gluon PDF $g(x, Q)$ in various $x$ ranges (for $Q^{2}=10 \mathrm{GeV}^{2}$ ), and $\chi^{2}$ for typical experimental data sets that are used in the PDF analysis. In this study, we compute $\cos \varphi$ for the experiments from the CT10 analysis that are listed in Table 4 . In the figures, we refer to each experiment by its numerical ID that is shown in the left column of Table 4 .

The $\cos \varphi$ values between the gluon PDF at a given $x$ value and $\chi^{2}$ for each experiment are plotted as two-dimensional contour plots for CT10 NLO PDFs [255] in the left panel of Fig. [11, and for MSTW' 08 NLO PDFs [262] in the right panel. The horizontal axis indicates the range of $x$ in $g(x, Q)$. The vertical axis indicates the ID of the experiment. At the bottom of the figure, we show the color legend adopted to draw the contour plots. The color legend is chosen so as to emphasize only cells with large correlation ( $\cos \varphi>0.5$, dark yellow-red colors) or large anticorrelation ( $\cos \varphi<-0.5$, blue colors). The regions with $|\cos \varphi|<0.5$ are filled with a light-yellow color. The $\chi^{2}$ values for each data set are computed according to Eqs. (66) and (69) using the CTEQ fitting code for both CT10 and MSTW PDF sets.

Visual inspection of two panels of Fig. 11 reveals both similarities and differences in the pattern of correlations of the gluon PDF in the CT10 and MSTW PDF sets. In the case of the CT10 PDF (left panel), the gluon PDF has a pronounced anti-correlation (blue spots) with HERA charm and bottom SIDIS production data sets (experiments $140,143,145,156,157$ ) at $x<0.1$, as well as with Tevatron inclusive jet production data sets (experiments $504,505,514$, and 515) at $x>0.05$. Some correlations (brown and red spots) are also observed, but they are not as pronounced as the anti-correlations. Weaker (anti-)correlations can be noticed with the NMC $F_{2}^{p}$, CDHSW $F_{2}^{p}$, and E605 pp Drell-Yan process data, corresponding to experiments 103, 108, and 201.

While the gluon PDF of the MSTW'08 set (right panel of Fig. 11) also shows an (anti-)correlation with the heavy-quark DIS and jet production data, the overall pattern of the correlations is somewhat different from the CT10 case. Here, the gluon PDF is mostly correlated with high- $x$ jet production (experiments 504, 505,514, and 515), while it is either correlated or anti-correlated with heavy-quark DIS experiments (experiments 140, 143, 145, 156, 157). In addition, we observe significant (anti-)correlations with the combined HERA DIS data set ( $\mathrm{ID}=159$ ) and fixed-target DIS experiments ( $\mathrm{ID}=101-124$ ) that are not seen in the CT10 panel.

We now turn to the correlations of the gluon and $u$-quark PDFs with $\chi^{2}$ values in individual bins of Tevatron inclusive jet and dijet production data. For this purpose, we represent $\chi^{2}$ for one experimental data set in Eq. 69 as a sum of contributions $\chi_{i}^{2}$ from individual data points $i$ :

$$
\begin{equation*}
\chi^{2}=\sum_{i=1}^{N_{e}} \chi_{i}^{2}, \tag{74}
\end{equation*}
$$

where

$$
\begin{equation*}
\chi_{i}^{2}=\frac{D_{i}-T_{i}}{\alpha_{i}} \sum_{j=1}^{N_{e}}\left\{\delta_{i j}-\frac{D_{j}-T_{j}}{\alpha_{j}} \sum_{k, k^{\prime}=1}^{K} \frac{\beta_{k i}}{\alpha_{i}} A_{k k^{\prime}}^{-1} \frac{\beta_{k^{\prime} j}}{\alpha_{j}}\right\} . \tag{75}
\end{equation*}
$$

Each contribution $\chi_{i}^{2}$ accounts for the effect of correlated systematic shifts through the term that includes $A_{k k^{\prime}}^{-1}$ on the right-hand side of Eq. 75 . Again, the constraining power of each point is determined both


Fig. 11: Correlation between the gluon distribution from CT10 NLO (left) and MSTW2008 NLO (right) PDF sets and $\chi^{2}$ for the experiments used in the CT10 global QCD analysis. The color of each cell indicates the value of $\cos \varphi$ according to the included legend. The ID's of individual experiments are listed in Table 4

| ID | Experimental data set |
| :---: | :---: |
| 159 | Combined HERA1 NC and CC DIS [263] |
| 101 | BCDMS $F_{2}^{p}$ [264] |
| 102 | BCDMS $F_{2}^{d}$ [265] |
| 103 | NMC $F_{2}^{p}$ [266] |
| 104 | NMC $F_{2}^{d} / F_{2}^{p}$ [266] |
| 108 | CDHSW $F_{2}^{p}$ [267] |
| 109 | CDHSW $F_{3}^{p}$ [267] |
| 110 | CCFR $F_{2}^{p}$ [268] |
| 111 | CCFR $x F_{3}^{p}$ [269] |
| 124 | NuTeV neutrino dimuon SIDIS [270] |
| 125 | NuTeV antineutrino dimuon SIDIS [270] |
| 126 | CCFR neutrino dimuon SIDIS [271] |
| 127 | CCFR antineutrino dimuon SIDIS [271] |
| 140 | H1 $F_{2}^{c}$ [272] |
| 143 | H1 $\sigma_{r}^{c}$ for $c \bar{c}$ [273, 274] |
| 145 | H1 $\sigma_{r}^{b}$ for $b \bar{b}$ [273, 274] |
| 156 | ZEUS $F_{2}^{c}$ [275] |
| 157 | ZEUS $F_{2}^{c}$ [276] |
| 201 | E605 Drell-Yan process, $\sigma(p A)$ [277] |
| 203 | E866 Drell Yan process, $\sigma(p d) /(2 \sigma(p p))$ [278] |
| 204 | E866 Drell-Yan process, $\sigma(p p)$ [279] |
| 225 | CDF Run-1 $W$ charge asymmetry [280] |
| 227 | CDF Run-2 $W$ charge asymmetry [281] |
| 231-234 | DØ Run-2 W charge asymmetry [282] |
| 260 | DØ Run-2 Z rapidity distribution [283] |
| 261 | CDF Run-2 Z rapidity distribution [284] |
| 504 | CDF Run-2 inclusive jet production [285] |
| 505 | CDF Run-1 inclusive central jet production [286] |
| 514 | DØ Run-2 inclusive jet production [287] |
| 515 | DØ Run-1 inclusive jet production [288] |

Table 4: Experimental data sets examined in this analysis.


Fig. 12: Correlation cosine between $\chi_{i}^{2}$ in each $p_{T}$ bin from D $\emptyset$ Run- 2 inclusive jet production and gluon and $u$ quark distributions from CT10 and MSTW 2008 NLO sets. The horizontal axis refers to the $x$ value in the PDF. The vertical axis indicates the numerical ID of the experimental bin for which $\chi^{2}$ is computed. The ID for each bin is indicated as $100 i_{y}+i_{p_{T}}$, where $i_{y}=1, \ldots 6$ and $i_{p_{T}}$ are the ID's of the corresponding rapidity interval and the $p_{T}$ interval, respectively.


Fig. 13: Correlation cosine between $\chi_{i}^{2}$ in each $m_{j j}$ bin from D $\emptyset$ Run-2 dijet production and gluon and $u$ quark distributions from CT10 and MSTW 2008 NLO sets. The horizontal axis refers to the $x$ value in the PDF. The vertical axis indicates the numerical ID of the experimental bin for which $\chi^{2}$ is computed. The ID for each bin is indicated as $100 i_{y_{\max }}+i_{m_{j j}}$, where $i_{y_{\max }}=1, . ., 6$ and $i_{m_{j j}}$ are the ID's of the corresponding intervals in $y_{\max }$ and $m_{j j}$, respectively.
by the value of $|\cos \varphi|$ and the magnitude of $\chi_{i}^{2}$, with the latter being comparable to unity for the majority of the data points.

For D $\emptyset$ Run-2 single-inclusive jet cross sections [287], we plot the $\cos \varphi$ values for the gluon and $u$-quark PDFs, with $\chi_{i}^{2}$ computed for each bin of the jet's transverse momentum $p_{T}$ and rapidity $y$. The resulting contour plots are shown in Fig. 12. Similarly, for DØ Run-2 dijet cross sections [289], Fig. 13 shows the contour plots of $\cos \varphi$ for $\chi_{i}^{2}$ in the bins of of dijet invariant mass $m_{j j}$ and maximal absolute rapidity $|y|=\max \left(\left|y_{1}\right|,\left|y_{2}\right|\right)$ of the dijets. In both figures, theory cross sections are computed at NLO (without threshold resummation corrections) with the FASTNLO code [290, 291], using the settings described in Section 13. The same color legend as in Fig. 11 is used. Similar patterns of correlations were found with the CDF Run-2 inclusive jet data (not shown).

The upper panels in both figures show $\cos \varphi$ for CT 10 NLO and MSTW' 08 NLO gluon PDFs. The correlated experimental errors modify the correlations by smearing the $\cos \varphi$ distribution. The pattern of $\cos \varphi$ indicates clearly that the (di)jet data are very sensitive to the gluon at $x$ above 0.01 . However, the correlation is weaker for the CT10 gluon PDF (left panel) then for MSTW'08 PDF (right panel), suggesting that the importance of the constraints on the gluon PDF from the jet data is not the same in two fits. In addition, the MSTW'08 $u$-quark PDF shows mild (anti-)correlation with both single-inclusive jet data and dijet data, as can be observed in the right lower panels in Figs. 12 and 13 . No pronounced (anti-)correlations with the $u$-quark PDF or other quark PDFs of physical flavors are observed for the CT10 set, shown in the lower left panels.

The contour plots confirm the expectation that the inclusive jet data play an important role in constraining the gluon PDF. While the constraints are strongest at $x>0.1$, they extend down to $x$ as low as 0.05 for both CT10 and MSTW sets, as can be observed in Figs. 12 and 13 . The gluon PDF is sensitive to constraints from heavy-quark semi-inclusive DIS production at even lower $x$ values, cf. Fig. 11. As the HERA data on heavy-quark DIS production continue to improve, it will play an increasingly important role in constraining the low- $x$ gluon density.

While the patterns of PDF-induced correlations are visually similar for the CT10 and MSTW'08 sets, they are not completely identical. Constraints on the gluon PDF from Tevatron jet production may not be as strong in the CT10 fit as in the MSTW'08 fit, according to Figs. 12 and 13 It remains to be investigated what causes the observed differences between CT10 and MSTW sets in the correlations involving the gluon PDF. Several features are different in these fits, including different heavy-quark DIS schemes, choice of experimental data sets, PDF parametrizations, and radiative contributions in theoretical cross sections. A combination of these effects may indirectly affect the strength of the constraints imposed on the gluon density by the collider jet data.

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## 8. PDF CONSTRAINTS FROM ELECTROWEAK VECTOR BOSON PRODUCTION AT THE LHC ${ }^{10}$


#### Abstract

We present a study of the impact of the recent $W$ and $Z$ measurements from ATLAS, CMS and LHCb on parton distribution functions. We show that the NNPDF2.1 NNLO predictions are consistent with all the new data, but that these provide significant further constraints on the light quarks and antiquarks


[^124]at medium and small- $x$. We conclude that these data already have the potential to play a useful role in future global PDF analyses.

### 8.1 LHC measurements sensitive to PDFs

The LHC has already provided an impressive set of measurements which are sensitive to parton distributions: inclusive jet and dijet data [292, 293, 294], electroweak vector boson production [295, 296, 297, 298, 299, 300] (both inclusive and in association with heavy quarks [301]) and direct photon production [302, 303]. The purpose of this contribution is to quantify the impact on PDFs of a subset of these data, the $W$ and $Z$ inclusive production measurements. In this first section we will review the status of LHC data relevant for PDF determination and then in the next section we will study how the $W, Z$ data impact on the NNPDF analysis.

Let's begin this short review of LHC data with electroweak vector boson production. ATLAS has measured the $W$ lepton and $Z$ rapidity distributions using the 2010 data ( $36 \mathrm{pb}^{-1}$ ) and determined the full covariance matrix of correlated experimental uncertainties [295]. This measurement supersedes the original muon asymmetry measurement from $W$ decays [296], for which the covariance matrix was not available. The CMS collaboration has presented a preliminary measurement of the muon asymmetry with 2011 data ( $234 \mathrm{pb}^{-1}$ ) [297] which supersedes the 2010 data [298]. In addition it has presented a measurement of the normalized $Z$ rapidity distribution using 2010 data [299]. In neither of these two measurements has the full covariance matrix been made available. Finally, the LHCb Collaboration has presented preliminary results for the $Z$ rapidity distribution, $W$ lepton asymmetry and W lepton charge ratio using 2010 data [300].

| Data Set | Ref. | $N_{\text {dat }}$ | $\left[\eta_{\text {min }}, \eta_{\text {max }}\right]$ | $\left\langle\sigma_{\text {stat }}\right\rangle(\%)$ | $\left\langle\sigma_{\text {sys }}\right\rangle$ (\%) | $\left\langle\sigma_{\text {norm }}\right\rangle$ (\%) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ATLAS W,Z $36 \mathrm{pb}^{-1}$ | [295] | 30 | [0, 3.2] | 1.9 | 1.7 | 3.4 |
| ATLAS $W^{+} 36 \mathrm{pb}^{-1}$ | [295] | 11 | [0, 2.4] | 1.4 | 1.3 | 3.4 |
| ATLAS $W^{-} 36 \mathrm{pb}^{-1}$ | [295] | 11 | [0, 2.4] | 1.6 | 1.4 | 3.4 |
| ATLAS $Z 36 \mathrm{pb}^{-1}$ | [295] | 8 | [0, 3.2] | 2.8 | 2.4 | 3.4 |
| CMS $Z$ rapidity $36 \mathrm{pb}^{-1}$ | [299] | 35 | [0, 3.6] | 12.3 | - | 0 |
| CMS muon asymmetry $234 \mathrm{pb}^{-1}$ | [297] | 11 | [0, 2.4] | 1.7 | 3.1 | 0 |
| LHCb $Z$ rapidity $36 \mathrm{pb}^{-1}$ | [300] | 5 | [2, 4.5] | 20 | 5 | 3.4 |
| LHCb $W$ lepton asymmetry $36 \mathrm{pb}^{-1}$ | [300] | 5 | [2, 4.5] | 16 | 21 | 0 |

Table 5: The number of data points, kinematical coverage and average statistical, systematic and normalization percentage uncertainties for each of the experimental LHC $W$ and $Z$ datasets considered in the present analysis. For the CMS $Z$ rapidity data, the systematic uncertainty is included in the statistical uncertainty: there is no normalization uncertainty because these data are normalised to the total cross-section.

The kinematical coverage of each of the various LHC $W$ and $Z$ dataset with the corresponding average experimental uncertainties for each dataset are summarized in Table5. As we can see the LHC electroweak data span a large range in rapidity up to $\eta=4.5$. Each of the three processes considered, $W^{+}, W^{-}$and $Z$ is sensitive to different partonic subprocesses.

There are other LHC datasets potentially sensitive to PDFs. Jet production from the Tevatron has been a very important measurement not only to constrain the gluon at high $x$, but in determining the strong coupling from a global PDF analysis [304, 305]. Similar constraints are expected from the LHC jet data, extended into a wider kinematical range. From the $2010\left(36 \mathrm{pb}^{-1}\right)$ dataset inclusive jet and dijet production has been measured by both CMS [292, 293] and ATLAS [294], however only for ATLAS is the full experimental covariance matrix available. The LHC inclusive jet data can be treated within a global analysis framework using tools like FastNLO or APPLgrid [306]. Since the full NNLO corrections to the inclusive jet production are unknown, jet data in a NNLO analysis can be included only within some approximation: for example with NNLO PDF evolution and coupling running but with NLO matrix elements, or else with NLO matrix elements supplemented with Sudakov estimates of the

NNLO corrections. Another LHC measurement that has the potential to constrain the gluon PDFs is prompt photon production from ATLAS [302] and CMS [303]: its consistency with NLO QCD and their impact on the NNPDF2.1 PDFs will be discussed in detail in Ref. [307].

### 8.2 PDF constraints from LHC $W$ and $Z$

Until recently all available NNPDF sets [308, 309, 261, 310, 311, 312, 313] were based on non-LHC data. NNPDF2.2 [314] was the first set to include LHC data, the $W$ lepton asymmetry from ATLAS and CMS [298, 296]. However now these two datasets are outdated, the first because now the full correlation matrix of the $W$ and $Z$ lepton distributions is available, and the second because data from higher luminosities is also available. So we have chosen to continue to use as our baseline the NNPDF2.1 NNLO set.

We now study the impact of the latest LHC $W$ and $Z$ data on the NNPDF parton distributions. All our theoretical NNLO predictions will be computed with DYNNLO [315] with the same cuts and settings as in the respective measurements. The impact of the new data will be quantified using the reweighting method of Refs. [316, 314] applied to the $N_{\text {rep }}=1000$ replicas of the NNPDF2.1 NNLO set.

To begin with, we have computed the $\chi^{2}$ for each of the datasets in Table 5 for the most recent NNLO PDF sets currently available on LHAPDF: NNPDF2.1, MSTW08 [262], ABKM09 [317], HERAPDF1.5 [318] and JR09 [319]. When available, we use the full experimental covariance matrix. Normalization uncertainties are included using the $t_{0}$ method [320]. This is important specially for the treatment of the ATLAS differential distributions where normalization uncertainties are comparable to the statistical and systematic uncertainties (See Table 5).

The results are summarized in Table 6. For the ATLAS $W$ and $Z$ lepton distributions we show the results both for the total dataset and the individual subsets, where in the latter case cross-correlations between subsets have been neglected. In all cases the theoretical NNLO predictions have been obtained with DYNNLO as discussed above. We can see that none of these PDF sets describes the ATLAS and CMS data perfectly, although NNPDF2.1 and HERAPDF1.5 give probably the best description, while ABKM09 and JR09 are significantly worse. All five sets give a reasonable description of the LHCb data within their large uncertainties.

| Dataset | $\chi^{2}$ NNPDF2.1 | $\chi^{2}$ MSTW08 | $\chi^{2}$ ABKM09 | $\chi^{2}$ JR09 | $\chi^{2}$ HERAPDF1.5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ATLAS | 2.7 | 3.6 | 3.6 | 5.0 | 2.0 |
| ATLAS $W^{+} 36 \mathrm{pb}^{-1}$ | 5.7 | 6.5 | 11.4 | 5.4 | 5.3 |
| ATLAS $W^{-} 36 \mathrm{pb}^{-1}$ | 2.5 | 4.1 | 5.4 | 8.0 | 6.4 |
| ATLAS $Z 36 \mathrm{pb}^{-1}$ | 1.8 | 3.7 | 4.2 | 6.5 | 2.9 |
| CMS | 2.0 | 3.0 | 2.8 | 3.6 | 2.8 |
| CMS $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.9 | 2.9 | 2.7 | 2.0 | 3.0 |
| CMS muon asymmetry $234 \mathrm{pb}^{-1}$ | 2.0 | 3.4 | 3.0 | 8.7 | 2.1 |
| LHCb | 0.8 | 0.7 | 1.2 | 0.4 | 0.6 |
| LHCb $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.1 | 0.7 | 0.8 | 0.6 | 0.8 |
| LHCb $W$ lepton asymmetry $36 \mathrm{pb}^{-1}$ | 0.5 | 0.6 | 1.6 | 0.2 | 0.5 |

Table 6: Comparison between LHC $W$ and $Z$ data and the most recent NNLO PDFs. For each PDF set we provide the $\chi^{2} / d o f$ between data and theory predictions, computed using the $t_{0}$-method.

For the ATLAS data, we would like to emphasize the importance of properly taking into account the correlations between datasets, specially the normalization: the description of the individual $W^{+}$, $W^{-}$and $Z$ datasets is always worse than the overall description because of these cross-correlations. For the CMS $Z$ rapidity distribution we find that the fixed order NNLO description seems rather worse than the NLO+LL prediction implemented in POWHEG [299]: the origin of this difference should be investigated in future studies.

We now discuss the impact of these LHC EW data into the NNPDF2.1 NNLO PDFs [313]. In Table 7 we summarize the initial $\chi^{2}$ for each dataset, the $\chi^{2}$ after reweighting, $\chi_{\mathrm{rw}}^{2}$. We find excellent agreement with all the LHC electroweak measurements after reweighting. Some comparisons between data and theory for a selected observables are shown in Fig. 14. From top to bottom we show the comparison with ATLAS, CMS and LHCb data. In each case we have included all the most updated electroweak datasets from each collaboration.

In Table 7 we also show the effective number of replicas left after the reweighting, defined as in Ref. [316] using the Shannon entropy,

$$
\begin{equation*}
N_{\text {eff }} \equiv \exp \left\{\frac{1}{N_{\text {rep }}} \sum_{k=1}^{N_{\text {rep }}} w_{k} \ln \left(N_{\text {rep }} / w_{k}\right)\right\} \tag{76}
\end{equation*}
$$

In each case we have performed the reweighting separately for each of the experimental datasets individually, for the combined datasets from each experiment, and finally with all three combined together.

| Dataset | $\chi^{2}$ | $\chi_{\mathrm{rw}}^{2}$ | $N_{\text {eff }}$ |
| :---: | :---: | :---: | :---: |
| ATLAS | 2.7 | 1.2 | 16 |
| ATLAS $W^{+} 36 \mathrm{pb}^{-1}$ | 5.7 | 1.5 | 17 |
| ATLAS $W^{-} 36 \mathrm{pb}^{-1}$ | 2.5 | 1.0 | 205 |
| ATLAS $Z 36 \mathrm{pb}^{-1}$ | 1.8 | 1.1 | 581 |
| CMS | 2.0 | 1.2 | 56 |
| CMS $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.9 | 1.4 | 223 |
| CMS muon asymmetry $234 \mathrm{pb}^{-1}$ | 2.0 | 0.4 | 200 |
| LHCb | 0.8 | 0.8 | 972 |
| LHCb $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.1 | 1.0 | 962 |
| LHCb $W$ lepton asymmetry $36 \mathrm{pb}^{-1}$ | 0.8 | 0.5 | 961 |
| All data combined | 2.1 | 1.2 | 4 |

Table 7: The impact of LHC electroweak measurements on the NNPDF2.1 NNLO PDFs. For each dataset we show the initial $\chi^{2}$, the $\chi^{2}$ after reweighting these particular dataset and the effective number of replicas $N_{\text {eff }}$ in this case. We show both the results for individual datasets as well as for the combined impact of all datasets within the same experiment. All the results have been computed starting with $N_{\text {rep }}=1000$ replicas.

When all the datasets are taken together, the initial $\chi^{2}=2.1$, already quite reasonable is reduced down to $\chi_{\mathrm{rw}}^{2}=1.2$, thus obtaining a very good overall description of all the most recent LHC electroweak data. The effective number of replicas for all combined datasets is only $N_{\text {eff }}=4$ however: from this we conclude that to determine the combined impact of these data on PDFs would require many more replicas (around 25,000 in fact, to obtain reasonable statistical accuracy), or, more practically, a new fit. Note that the fact that the total effective number of replicas for the whole dataset is rather smaller than that of any individual subset confirms their mutual compatibility and the lack of any appreciable tension. Comparing the effective number of replicas for the individual datasets, the most constraining data are the ATLAS $W$ and $Z$ distributions, specially the very precise $W^{+}$data. On the other hand the LHCb data have a rather small impact.

Let us now examine how various PDFs change when new experiments are added. In particular we show in Fig. 15 the NNPDF2.1 NNLO $d\left(x, Q^{2}\right)$ and $\bar{u}\left(x, Q^{2}\right)$ PDFs at $Q^{2}=M_{W}^{2}$ as ratios to the central value before including the new data. As described above, we put together all the data from a given experiment. As can be seen, the ATLAS data give a moderate reduction in PDF uncertainties, and a somewhat softer small- $x$ sea quarks, although the old and new PDFs agree at the 1 -sigma level. For CMS the central values for the old and new PDFs are unchanged with a moderate error reduction at medium- $x$. Finally, for LHCb the PDF uncertainties are almost unaffected, due to the low constraining power of these datasets.


Fig. 14: Comparison between data and theory before and after reweighting for NNPDF2.1 NNLO compared to the various LHC EW datasets considered. From top to bottom we show comparisons with ATLAS ( $W^{+}$lepton $Z$ rapidity distributions), CMS ( $W$ lepton asymmetry and $Z$ rapidity distribution) and LHCb data (same as CMS). For the ATLAS data the error bars include statistical and systematic uncertaintes, but not the normalization uncertainties.

### 8.3 Conclusions

In this contribution we have quantified the impact of the most updated LHC electroweak data on the NNPDF2.1 NNLO parton distributions. NNPDF2.1 provides a reasonable description of all these datasets even before their impact on the PDFs is included. We find that all the datasets are mutually consistent, with no obvious tensions. The PDF uncertainties for the light quarks and antiquarks at medium and small- $x$ are moderately reduced. The ATLAS $W, Z$ data seem to prefer a softer small- $x$ sea. It is clear from our results that the LHC $W$ and $Z$ data should play an important part in any future PDF global fit.

## Acknowledgments

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Fig. 15: Comparison between the NNPDF2.1 NNLO parton distributions before and after reweighting with the various LHC EW datasets considered. From top to bottom: ATLAS, CMS and LHCb data, where the left column we show the ratio of the $d$ quark PDF and in the right column the ratio of the $\bar{u}$ quark PDF to their central values before reweighting.


Fig. 16: $F_{L}$ vs. $Q^{2}$ for the HERA combined measurements from H 1 and ZEUS [321].

## 9. HEAVY QUARK PRODUCTION IN THE ACOT SCHEME AT NNLO AND $\mathbf{N}^{3} \mathbf{L O}^{11}$


#### Abstract

We extend the ACOT scheme for heavy quark production to NNLO and $\mathrm{N}^{3} \mathrm{LO}$ for the structure functions $F_{2}$ and $F_{L}$ in deep-inelastic scattering (DIS). We use the fully massive ACOT scheme up to NLO, and estimate the dominant heavy quark mass effects at the higher orders using the massless Wilson coefficients together with a generalized slow-rescaling prescription. We present results for $F_{2}$ and $F_{L}$ showing the effect of the higher orders and the contributions from the heavy flavors.


### 9.1 INTRODUCTION

The production of heavy quarks in high energy processes has become an increasingly important subject of study both theoretically and experimentally. The theory of heavy quark production in perturbative Quantum Chromodynamics ( pQCD ) is more challenging than that of light parton (jet) production because of the additional heavy quark mass scale. The correct theory must properly take into account the changing role of the heavy quark over the full kinematic range of the relevant process from the threshold region (where the quark behaves like a typical "heavy particle") to the asymptotic region (where the same quark behaves effectively like a parton, similar to the well known light quarks $\{u, d, s\}$ ).

With the ever-increasing precision of experimental data and the progression of theoretical calculations and parton distribution function (PDF) evolution to next-to-next-to-leading order (NNLO) of QCD, there is a clear need to implement the heavy quark schemes at this order and beyond. The most important case is arguably the heavy quark treatment in inclusive deep-inelastic scattering (DIS) since the very precise HERA data for DIS structure functions and cross sections form the backbone of any modern global analysis of PDFs. Here, the heavy quark structure functions contribute up to $30 \%$ or $40 \%$ to the inclusive structure functions at small momentum fractions $x$. Extending the heavy quark schemes to higher orders is relevant for extracting precision PDFs, and hence for accurate predictions of observables at the LHC.

An example where higher order corrections are particularly important is the longitudinal structure function $F_{L}$ in DIS. The leading order $\mathcal{O}\left(\alpha_{s}^{0}\right)$ contributions to this structure function vanishes for massless quarks due to helicity conservation (Callan-Gross relation). Since the first unsuppressed contribution to $F_{L}$ is at next-to-leading order, the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ corrections are more important than for $F_{2}$. In Fig. 16 we show the preliminary results for the $F_{L}$ measurement from the H1 and ZEUS experiments [321]. In Fig. 17 displays sample Feynman diagrams at the various orders. Producing an accurate

[^125]

Fig. 17: Example Feynman diagrams contributing to DIS heavy quark production (from left): LO $\mathcal{O}\left(\alpha_{S}^{0}\right)$ quark-boson scattering $Q V \rightarrow Q$, NLO $\mathcal{O}\left(\alpha_{S}^{1}\right)$ boson-gluon scattering $g V \rightarrow Q \bar{Q}$, NNLO $\mathcal{O}\left(\alpha_{S}^{2}\right)$ boson-gluon scattering $g V \rightarrow g Q \bar{Q}$ and $\mathrm{N}^{3} \mathrm{LO} \mathcal{O}\left(\alpha_{S}^{3}\right)$ boson-gluon scattering $g V \rightarrow g g Q \bar{Q}$.
prediction for $F_{L}$ is a challenge, particularly in the region of low $Q^{2}$ and small $x$.
In this paper, we will briefly outline the method we used to incorporate the higher order terms, the key elements of the ACOT scheme, and the treatment of the heavy quark masses. We then present results for the $F_{2}$ and $F_{L}$ neutral current DIS structure functions.

### 9.2 THE ACOT SCHEME AND ITS EXTENSION BEYOND NLO



Fig. 18: Comparison of schemes for $F_{2}^{c}$ at $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number Scheme (FFNS), and Zero-Mass Variable-Flavor-Number-Scheme (ZM-VFNS). The ACOT and S-ACOT results are virtually identical.

The ACOT scheme [322, 323] is based upon the factorization theorem for heavy quarks[324]; hence, it is valid at any order of perturbation theory. The factorization proof ensures that the ACOT scheme can be applied throughout the full kinematic regime, and that there is a smooth transition from a massless result $(m=0)$ to the heavy-mass decoupling limit $(m \rightarrow \infty)$.

In the limit where the quark $Q$ of mass $m$ is relatively heavy compared to the characteristic energy scale ( $\mu \lesssim m$ ), the ACOT result naturally reduces to the Fixed-Flavor-Number-Scheme (FFNS). In the FFNS, the heavy quark is treated as being extrinsic to the hadron, and there is no corresponding heavy quark PDF, $f_{Q}(x, \mu)=0$. Conversely, in the limit where the quark mass is relatively light $(\mu \gtrsim m)$, the ACOT result reduces to the $\overline{M S}$ Zero-Mass Variable-Flavor-Number-Scheme (ZM-VFNS) exactlywithout any finite renormalizations. In this limit, the quark mass $m$ no longer plays any dynamical role; it serves purely as a regulator. This feature is presented in Fig. 18 where we can see that the ACOT scheme precisely matches the results of the FFNS and ZM-VFNS schemes in their respective limits.

Additionally Fig. 18 shows the results obtained within the Simplified-ACOT scheme (SACOT) [325]. The S-ACOT scheme drops the heavy quark mass dependence for the hard-scattering


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Additionally Fig. 18 shows the results obtained within the Simplified-ACOT scheme (SACOT) [325]. The S-ACOT scheme drops the heavy quark mass dependence for the hard-scattering


Fig. 19: $F_{L}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right). The three lines show the mass effects via the scaling variable: $n=\{0,1,2\}$, (Red, Green, Blue). We observe the effect of the $n$-scaling is negligible except for small $x$ and $Q$ values.
processes with incoming heavy quarks or with internal on-shell cuts on a heavy quark line. The S-ACOT scheme is not an approximation; it is an exact renormalization scheme, extensible to all orders. Note, the ACOT and S-ACOT results agree throughout the kinematic region.

### 9.21 Beyond NLO

While there is no conceptual difficulty with extending the ACOT scheme beyond NLO, the fully massive Wilson coefficients have yet to be computed ${ }^{[12}$ However massless calculations of NNLO and even $\mathrm{N}^{3} \mathrm{LO}$ for $F_{2}$ and $F_{L}$ structure functions are available $\sqrt{13}$

The question is: can we use these results, together with the knowledge that ACOT reduces to the massless $\overline{M S}$ (ZM-VFNS) for $m \rightarrow 0$, to estimate mass effects at NNLO and $\mathrm{N}^{3} \mathrm{LO}$ ? Obviously we cannot restore the fully massive ACOT result from the massless limit, but we can try to extract the dominant higher order contributions. There are two ways in which mass effects enter the calculation. The first is "dynamically" through the mass dependent Wilson coefficients. The second is "kinematically" via the restricted phase space. Comparisons using the fully massive results at NLO suggest that the kinematic mass effects are dominant, and that much of this dependence can be obtained with a rescaling of the Bjorken $x$ variable. We introduce a generalized rescaling $x \rightarrow x\left[1+(n m / Q)^{2}\right]$ where $n=0$ is the massless result, $n=1$ is the original Barnett[329] rescaling, and $n=2$ is the $\chi$-rescaling [330].

Thus, our strategy is as follows. We use the fully massive ACOT result to NLO [331], and add to this the massless NNLO and $\mathrm{N}^{3} \mathrm{LO}$ contributions using the generalized rescaling prescription. By varying $n$, we can investigate the influence of the kinematic mass in our results. We argue that the massless Wilson coefficients at NNLO and $\mathrm{N}^{3} \mathrm{LO}$, together with the generalized rescaling prescription provide a good approximation of the exact result. At worst, the error is of order $\alpha \alpha_{S}^{2} \times\left[m^{2} / Q^{2}\right]$, and comparative studies at NLO suggest the error is less. ${ }^{[14}$ For example, in Fig. 19 we display the results of $F_{L}$ for $n=\{0,1,2\}$. The effects of the detailed mass dependence is most noticeable for low $Q^{2}$ and small $x$. While the massless scaling result $(n=0)$ does deviate from the other curves, comparing the $n=1$ and $n=2$ curves we observe the details of the mass rescaling are relatively small. While this is not a proof ${ }_{[15}^{15}$ this result does give us confidence that the mass effects are under control.


Fig. 20: Fractional contribution for each quark structure function $F_{2, L}^{i}$ for each flavor $i=\{u, d, s, c, b\}$ for (a) $F_{2}^{i}$ and (b) $F_{L}^{i}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for the ACOT- $\chi$ scheme.

### 9.3 RESULTS

In Fig. 20 we display the fractional contributions to the structure functions $F_{2}$ and $F_{L}$. At larger values of $x$ and low $Q$, we observe that the heavy flavor contributions are minimal. For example, for $x=10^{-1}$, we see that the $u$-quark structure function $F^{u}$ comprises $\sim 80 \%$ of the total structure function. In contrast, at $x=10^{-5}$ and large $Q$ we see that the contributions of the $u$ and $c$ quarks are comparable (as they couple with a factor 4/9), and the $d$ and $s$ quarks contributions are comparable (as they couple with a factor $1 / 9$ ).

Figure 20 also shows how the $\chi$-rescaling introduces a damping of the heavy quark contributions as we move from large $Q^{2}$ values to smaller values. The $\chi$-rescaling ensures the heavy quarks $(c, b)$ are appropriately suppressed for low $Q^{2}$ scales.

In Fig. 21a we display the results for $F_{2}$ vs. $Q$ computed at various orders; the ratio to the $\mathrm{N}^{3} \mathrm{LO}$ result is displayed in Fig. 21b For large $x$ (c.f. $x=0.1$ ) we find the perturbative calculations are particularly stable. We see that the LO result is within $20 \%$ of the others at small $Q$, and within $5 \%$ at large $Q$. The NLO is within $2 \%$ at small $Q$, and indistinguishable from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ for $Q$ values above $\sim 10 \mathrm{GeV}$. The NNLO and $\mathrm{N}^{3} \mathrm{LO}$ results are essentially identical throughout the kinematic range. For smaller $x$ values $\left(10^{-3}, 10^{-5}\right)$, the contributions of the higher order terms are slightly larger. Here, the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ coincide for $Q$ values above $\sim 5 \mathrm{GeV}$, but the NLO result can differ by $\sim 5 \%$ for low $Q^{2}$ scales.

In Fig. 22 we display the results for $F_{L}$ vs. $Q$ computed at various orders. In contrast to $F_{2}$, we find that NLO corrections are large; this is expected because the LO corrections to $F_{L}$ (which violate

[^126]
(a) $F_{2}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

(b) Ratio of $F_{2}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) compared to $F_{2}$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=$ $\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

Fig. 21: $F_{2}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$.
the Callan-Gross relation) are suppressed by $\left(m^{2} / Q^{2}\right)$ compared to the dominant gluon contributions which enter at NLO. Consequently, we observe that the LO result for $F_{L}$ receives large contributions from the higher order terms. Essentially, NLO is the first non-trivial order for $F_{L}$, and the subsequent contributions then converge. For example, at large $x$ (c.f. $x=0.1$ ) for $Q \sim 10 \mathrm{GeV}$ we find the NLO results yields $\sim 70 \%$ of the total, the NNLO is a $\sim 20 \%$ correction, and the $\mathrm{N}^{3} \mathrm{LO}$ is a $\sim 10 \%$ correction. For lower $x$ values $\left(10^{-3}, 10^{-5}\right.$ ) the convergence of the perturbative series improves, and the NLO results is within $\sim 10 \%$ of the $\mathrm{N}^{3} \mathrm{LO}$ result. Curiously, for $x=10^{-5}$ the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ roughly compensate each other so that the NLO and the $\mathrm{N}^{3} \mathrm{LO}$ match quite closely for $Q \gtrsim 2 \mathrm{GeV}$.

### 9.4 CONCLUSIONS

We have computed the $F_{2}$ and $F_{L}$ structure functions in the ACOT scheme at NNLO and $\mathrm{N}^{3} \mathrm{LO}$. The full mass dependence is computed to NLO, and the dominant mass effects for the higher orders are approximated using a generalized rescaling; the details of this rescaling are demonstrated to be small. This allows us to make detailed predictions throughout the kinematic range investigated by HERA, and we obtain a reasonable estimate of the uncertainty due to the higher order mass effects. Together with the precise HERA data, these calculations facilitate accurate determination of the PDFs which are the foundation of the LHC calculations.

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(a) $F_{L}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

(b) Ratio of $F_{L}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) compared to $F_{L}$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=$ $\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

Fig. 22: $F_{L}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$.

## Part IV

## PHENOMENOLOGICAL STUDIES OF OBSERVABLES AND UNCERTAINTIES

## 10. FINITE-WIDTH EFFECTS IN TOP-QUARK PAIR PRODUCTION AND DECAY AT THE LHC ${ }^{16}$


#### Abstract

We investigate finite-top-width effects in top-quark pair production by comparing NLO QCD predictions for $\mathrm{pp} \rightarrow$ WWb $\overline{\mathrm{b}}$ to corresponding $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow$ WWb $\bar{b}$ results in the narrow-top-width limit. Finite-top-width effects, which result from non-resonant and off-shell contributions, are discussed in detail for the case of the inclusive cross section (with experimental cuts) and for selected differential observables in the di-lepton channel.


### 10.1 INTRODUCTION

Top-quark pair production at hadron colliders allows for key tests of the Standard Model and represents an omnipresent background to Higgs-boson and new-physics searches. The very large t $\bar{t}$ samples from the Tevatron and the LHC, and the steadily increasing systematic precision call for a continu-

[^127]ous improvement of theory predictions ${ }^{17}$ In this context, a reliable theoretical description of experimental cuts and exclusive $t \bar{t}$ observables, which depend on details of the $\mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ final state, requires higher-order calculations for top-pair production and decay. The first NLO QCD predictions for $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}+X[335,336$, 337] have been obtained in the narrow-top-width limit, an approximation where the $2 \rightarrow 4$ particle process is factorised into on-shell $t \bar{t}$ production and (anti)top decays, taking into account spin correlations. In this framework, it was shown that NLO QCD effects in top-quark decays have a significant impact on the kinematic properties of final-state leptons and b-jets [335, 336, 337], and play an important role for top-mass measurements at the LHC [338]. More recently, NLO QCD predictions for the complete $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}+X$ process became available [25, 23], which include all effects related to the finite top-quark width, i.e. on- and off-shell intermediate top quarks, non-resonant contributions, and their interference with resonant t $\bar{t}$ production. Besides new evidence for the importance of NLO corrections to $t \bar{t}$ production and decay, these studies provided a first quantitative assessment of finite-width effects in the inclusive cross section. Applying a numerical $\Gamma_{\mathrm{t}} \rightarrow 0$ extrapolation to the $\mathrm{NLO} \mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ predictions, it was found that finite-topwidth contributions to the WWbb cross section at the Tevatron and the LHC ( 7 TeV ) range from 0.2 to 1 percent [25, 23], which is perfectly consistent with the expected order of magnitude ( $\Gamma_{\mathrm{t}} / m_{\mathrm{t}} \simeq 0.9 \%$ ) of finite-top-width effects in inclusive observables.

In this study, we pursue the investigation of finite-top-width effects by means of a tuned comparison of the $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ NLO calculation of Ref. [25] against the narrow-top-width approximation of Ref. [336]. This permits us, for the first time, to investigate $\Gamma_{\mathrm{t}}$-effects in different phenomenologically interesting regions of the $\mathrm{WWb} \overline{\mathrm{b}}$ phase space, where large off-shell and non-resonant contributions cannot be excluded a priori as in the case of inclusive observables.

### 10.2 NARROW-TOP-WIDTH APPROXIMATION AND FINITE-WIDTH EFFECTS

Let us start by recalling the main features of the NLO QCD calculations of $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ in narrow-top-width approximation [336] and $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ with finite-top-width effects [25]. For brevity, we denote them as $t \bar{t}$ and WWbb calculations, respectively. Both calculations implement leptonic W-boson decays in spin-correlated narrow-W-width approximation.

In the narrow-top-width limit of Ref. [336], top-quark resonances are approximated by

$$
\begin{equation*}
\lim _{\Gamma_{\mathrm{t}} / m_{\mathrm{t}} \rightarrow 0} \frac{1}{\left(p_{\mathrm{t}}^{2}-m_{\mathrm{t}}^{2}\right)^{2}+m_{\mathrm{t}}^{2} \Gamma_{\mathrm{t}}^{2}}=\frac{\pi}{m_{\mathrm{t}} \Gamma_{\mathrm{t}}} \delta\left(p_{\mathrm{t}}^{2}-m_{\mathrm{t}}^{2}\right), \tag{77}
\end{equation*}
$$

with delta functions that enforce the on-shell conditions, $p_{\mathrm{t}}^{2}=m_{\mathrm{t}}^{2}$, and are accompanied by $1 / \Gamma_{\mathrm{t}}$ factors. Contributions of $\mathcal{O}\left(\Gamma_{\mathrm{t}} / m_{\mathrm{t}}\right)$, i.e. terms that do not involve two resonant top propagators, are systematically neglected. The differential $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$ cross section is factorised into the $\mathrm{pp} \rightarrow \mathrm{t} \mathrm{\bar{t}}$ cross section times $\mathrm{t} \rightarrow \mathrm{Wb}$ partial decay widths, $\mathrm{d} \sigma=\left(\mathrm{d} \sigma_{\mathrm{t} \overline{\mathrm{t}}} \mathrm{d} \Gamma_{\mathrm{t}} \mathrm{d} \Gamma_{\overline{\mathrm{t}}}\right) / \Gamma_{\mathrm{t}}^{2}$, taking into account top-quark spin correlations. The LO and NLO predictions can be schematically expressed as

$$
\begin{align*}
\mathrm{d} \sigma_{\mathrm{LO}} & =\Gamma_{\mathrm{t}, \mathrm{LO}}^{-2}\left(\mathrm{~d} \sigma_{\mathrm{tt}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{0}\right), \\
\mathrm{d} \sigma_{\mathrm{NLO}} & =\Gamma_{\mathrm{t}, \mathrm{NLO}}^{-2}\left[\left(\mathrm{~d} \sigma_{\mathrm{tt}}^{0}+\mathrm{d} \sigma_{\mathrm{t} \mathfrak{t}}^{1}\right) \mathrm{d} \Gamma_{\mathrm{t}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{0}+\mathrm{d} \sigma_{\mathrm{tt}}^{0}\left(\mathrm{~d} \Gamma_{\mathrm{t}}^{1} \mathrm{~d} \Gamma_{\mathrm{t}}^{0}+\mathrm{d} \Gamma_{\mathrm{t}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{1}\right)\right], \tag{78}
\end{align*}
$$

where the superscripts 0 and 1 indicate tree-level quantities and NLO corrections, respectively. The NLO prediction involves three terms, where the corrections are applied either to $\mathrm{d} \sigma_{\mathrm{tt}}$ or to one of the decays. All ingredients of $\mathrm{d} \sigma_{\mathrm{LO}}$ and $\mathrm{d} \sigma_{\mathrm{NLO}}$ have to be evaluated with input parameters at the corresponding perturbative order. In particular, LO and NLO predictions must be computed using $\Gamma_{\mathrm{t}, \mathrm{LO}}$ and $\Gamma_{\mathrm{t}, \mathrm{NLO}}$ decay widths, as indicated in $\left.\boxed{78}\right|^{18}$ This guarantees that-up to higher-order corrections-the integration over

[^128]the phase space of each top decay in (78) is consistent with the branching fraction
\[

$$
\begin{equation*}
\frac{\int \mathrm{d} \Gamma_{\mathrm{t} \rightarrow \mathrm{~b} l \nu}}{\Gamma_{\mathrm{t}}}=\frac{\Gamma_{\mathrm{t} \rightarrow \mathrm{~b} l \nu}}{\Gamma_{\mathrm{t}}}=\mathrm{BR}(\mathrm{t} \rightarrow \mathrm{~b} l \nu) . \tag{79}
\end{equation*}
$$

\]

In this context, let us point out that a consistent inclusion of finite-W-width corrections-both in the scattering amplitudes and the $\Gamma_{\mathrm{t}}$ input parameters-is expected to lead to doubly-suppressed effects. This is due to the fact that, in the $\Gamma_{\mathrm{t}} \rightarrow 0$ limit, $\mathcal{O}\left(\Gamma_{\mathrm{W}}\right)$ corrections to the numerator and denominator of the branching fraction (79) cancel. Finite-W-width corrections are thus expected to produce very small effects of $\mathcal{O}\left(\frac{\Gamma_{\mathrm{W}} \Gamma_{\mathrm{t}}}{M_{\mathrm{w}} m_{\mathrm{t}}}\right)$ in inclusive observables. This justifies the use of the narrow-W-width approximation in combination with finite-top-width contributions, which is the approach adopted in Ref. [25], although in kinematic regions where finite- $\Gamma_{\mathrm{t}}$ effects become large also finite-W-width corrections [23] might become non-negligible.

The calculation of Ref. [25] provides a full description of $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ at order $\mathcal{O}\left(\alpha_{\mathrm{S}}^{3} \alpha^{2}\right)$. The top-quark width is incorporated into the complex top mass, $\mu_{\mathrm{t}}^{2}=m_{\mathrm{t}}^{2}-\mathrm{i} m_{\mathrm{t}} \Gamma_{\mathrm{t}}$, in the complex-mass scheme [339]. In this way, off-shell-top contributions are consistently described by Breit-Wigner distributions. Besides contributions with two intermediate top resonances, also singly- and non-resonant diagrams are taken into account, including interferences. A few representative tree diagrams are shown in Fig 23. The NLO WWbb̄ predictions involve factorisable corrections to doubly-resonant diagrams, which provide the off-shell extension of NLO corrections in $t \bar{t}$ approximation (78). In addition, there are non-factorisable corrections, where $t \bar{t}$ production and decay parts of the process are connected via exchange of QCD partons, and NLO corrections to singly- and non-resonant topologies. Further technical aspects are discussed in the original publications [336, 25].







Fig. 23: Representative LO diagrams of doubly-resonant (upper line), singly-resonant (first diagram in lower line), and non-resonant type (last two diagrams in lower line).

### 10.3 NUMERICAL RESULTS

### 10.31 Input parameters and setup

In the following we compare $\mathrm{t} \overline{\mathrm{t}}$ and $\mathrm{WWb} \overline{\mathrm{b}}$ predictions for $\mathrm{W}^{+}\left(\rightarrow \nu_{\mathrm{e}} \mathrm{e}^{+}\right) \mathrm{W}^{-}\left(\rightarrow \mu^{-} \bar{\nu}_{\mu}\right) \mathrm{b} \overline{\mathrm{b}}$ production at the Tevatron ( $\mathrm{p} \overline{\mathrm{p}}$ collisions at 1.96 TeV ) and the LHC ( pp collisions at 7 and 14 TeV ). These results are based on the same input parameters and cuts as in Ref. [25]. In NLO (LO) QCD we employ MSTW2008NLO (LO) parton distributions [262] and describe the running of the strong coupling constant $\alpha_{\mathrm{S}}$ with two-loop (one-loop) accuracy, including five active flavours. Contributions induced by the strongly suppressed bottom-quark density are neglected. For the gauge-boson and top-quark masses we use $m_{\mathrm{t}}=172 \mathrm{GeV}, M_{\mathrm{W}}=80.399 \mathrm{GeV}$, and $M_{\mathrm{Z}}=91.1876 \mathrm{GeV}$. The masses of all other quarks, including b-quarks, are neglected. In view of the negligibly small Higgs-mass dependence we adopt the $M_{\mathrm{H}} \rightarrow \infty$ limit, i.e. we omit diagrams involving Higgs bosons. The electroweak couplings are derived

| Collider | $\sqrt{s}[\mathrm{TeV}]$ | approx. | $\sigma_{\mathrm{tt}}[\mathrm{fb}]$ | $\sigma_{\mathrm{WWb}}[\mathrm{fb}]$ | $\sigma_{\mathrm{tt}} / \sigma_{\mathrm{WWb}}-1$ | Ref. [25] |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Tevatron | 1.96 | LO | $44.691(8)_{-12.58}^{+19.81}$ | $44.310(3)_{-12.49}^{+19.68}$ | $+0.861(19) \%$ | $+0.8 \%$ |
|  |  | NLO | $42.16(3)_{-2.91}^{+0.00}$ | $41.75(5)_{-2.63}^{+0.00}$ | $+0.98(14) \%$ | $+0.9 \%$ |
| LHC | 7 | LO | $659.5(1)_{-173.1}^{+261.8}$ | $662.35(4)_{-174.1}^{+263.4}$ | $-0.431(16) \%$ | $-0.4 \%$ |
|  |  | NLO | $837(2)_{-87}^{+42}$ | $840(2)_{-87}^{+41}$ | $-0.41(31) \%$ | $-0.2 \%$ |
| LHC | 14 | LO | $3306.3(1)_{-763.6}^{+1086}$ | $3334.6(2)_{-771.2}^{+1098.5}$ | $-0.849(7) \%$ | --- |

Table 8: Integrated $\nu_{\mathrm{e}} \mathrm{e}^{+} \mu^{-} \bar{\nu}_{\mu} \mathrm{b} \overline{\mathrm{b}}$ cross section in narrow-with approximation $\left(\sigma_{\mathrm{t} \overline{\mathrm{t}}}\right)$ and including finite-top-width effects $\left(\sigma_{\mathrm{WWb}} \overline{\mathrm{b}}\right)$. The relative error of the narrow-width approximation (sixth column) is compared to the prediction of Ref. [25] (seventh column). Factor-two scale variations in $\sigma_{\mathrm{tt}}$ and $\sigma_{\mathrm{Wwb} \overline{\mathrm{b}}}$ are shown as sub- and super-scripts, while statistical errors are given in parenthesis.
from the Fermi constant $G_{\mu}=1.16637 \times 10^{-5} \mathrm{GeV}^{-2}$ in the $G_{\mu}$-scheme, where the sine of the mixing angle and the electromagnetic coupling read $s_{\mathrm{w}}^{2}=1-M_{\mathrm{W}}^{2} / M_{\mathrm{Z}}^{2}$ and $\alpha=\sqrt{2} G_{\mu} M_{\mathrm{W}}^{2} s_{\mathrm{w}}^{2} / \pi$. For consistency, we perform the LO and NLO calculations using the top-quark widths $\Gamma_{\mathrm{t}, \mathrm{LO}}=1.4655 \mathrm{GeV}$ and $\Gamma_{\mathrm{t}, \mathrm{NLO}}=1.3376 \mathrm{GeV}$ [340], respectively. Since the leptonic W-boson decay does not receive NLO QCD corrections we employ the NLO W-boson width $\Gamma_{\mathrm{W}}=2.0997 \mathrm{GeV}$ everywhere.

Final-state quarks and gluons with pseudo-rapidity $|\eta|<5$ are converted into infrared-safe jets using the anti- $k_{\mathrm{T}}$ algorithm [341]. For the Tevatron (LHC) we set the jet-algorithm parameter $R=0.4$ (0.5) and apply the transverse-momentum and pseudo-rapidity cuts $p_{\mathrm{T}, \mathrm{b}-\mathrm{jet}}>20(30) \mathrm{GeV},\left|\eta_{\mathrm{b}-\mathrm{jet}}\right|<2.5$. Moreover, we require a missing transverse momentum of $p_{\mathrm{T}, \mathrm{miss}}>25(20) \mathrm{GeV}$ and charged leptons with $p_{\mathrm{T}, l}>20 \mathrm{GeV}$ and $\left|\eta_{l}\right|<2.5$.

For the renormalisation and factorisation scales we adopt the central value $\mu=m_{\mathrm{t}}$ and study factor-two variations of $\mu=\mu_{\mathrm{ren}}=\mu_{\mathrm{fact}}$, i.e. we compare predictions at $\mu / m_{\mathrm{t}}=0.5,1,2$. The scale variations are applied also to $\Gamma_{\mathrm{t}, \mathrm{NLO}}$, but not to $\Gamma_{\mathrm{W}}$.

### 10.32 Integrated cross section

Results for the integrated $\nu_{\mathrm{e}} \mathrm{e}^{+} \mu^{-} \bar{\nu}_{\mu} \mathrm{b} \overline{\mathrm{b}}$ cross sections and scale uncertainties at the Tevatron and the LHC are reported in Table 8. While the $\sigma_{\text {Wwb币 }}$ results for Tevatron and LHC at 7 TeV correspond to those of Ref. [25] ${ }^{19}$, the ones for LHC at 14 TeV as well as all $\sigma_{\mathrm{t} \bar{\epsilon}}$ predictions are new. Comparing all $\mathrm{WWb} \overline{\mathrm{b}}$ and $t \bar{t}$ predictions we find that finite-top-width effects never exceed one percent, both in LO and NLO. The statistical precision of the calculations permits us to assess the error of the NWA, $\sigma_{\mathrm{t} \overline{\mathrm{t}}} / \sigma_{\mathrm{WWbb}}-1$, with an accuracy of $1-3$ permille. At the Tevatron, the NWA overestimates the WWb $\bar{b}$ cross section by an amount very close to $\Gamma_{\mathrm{t}} / m_{\mathrm{t}} \simeq 0.9 \%$, both in LO and NLO. The error of the NWA at the 7 (14) TeV LHC ranges between 4 and 8 permille. As shown in the last column of Table 8 these finite-width effects are in very good agreement with the results of the $\Gamma_{\mathrm{t}} \rightarrow 0$ extrapolation in Ref. [25]. Similar results can be found also in Ref. [23].

[^129]
### 10.33 Differential distributions

The small finite-width corrections to the integrated cross section demonstrate that-in presence of standard LHC and Tevatron cuts-the NWA provides a fairly accurate description of inclusive WWb̄ production. It is thus interesting to investigate to which extent this conclusion applies to the various phenomenologically important regions of the WWb $\overline{\mathrm{b}}$ phase space. To this end we have compared $\mathrm{t} \overline{\mathrm{t}}$ and WWbb predictions for a few differential observables that are relevant for top-pair production, either as signal or as background to Higgs production or new physics. Note that we refrain from selecting kinematic variables like the top-quark invariant mass or imposing cuts of type $M_{\mathrm{Wb}}>200 \mathrm{GeV}$, which would lead to obvious enhancements of non-resonant contributions.

In Figs. 2427 we present predictions for some invariant-mass and transverse-momentum distributions, restricting ourselves to the case of the 7 TeV LHC. For each observable we display $t \bar{t}$ (dashed curves) and $\mathrm{WWb} \overline{\mathrm{b}}$ (solid curves) results in LO (blue) and NLO (red) approximation. Absolute predictions (left plots) are complemented by the ratios $\left(\mathrm{d} \sigma_{\mathrm{LO}}-\mathrm{d} \sigma_{\mathrm{NLO}}\right) / \mathrm{d} \sigma_{\mathrm{NLO}}$ (upper right plots) and $\left(\mathrm{d} \sigma_{\mathrm{t} \bar{t}}-\mathrm{d} \sigma_{\mathrm{WWb} \overline{\mathrm{b}}}\right) / \mathrm{d} \sigma_{\mathrm{WWb}}$ (lower right plots), which indicate the relative error of LO and narrow-width approximations w.r.t. the best predictions, i.e. NLO and WWb $\overline{\mathrm{b}}$.


Fig. 24: Distribution in the transverse momentum of the harder b-jet at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb $\overline{\mathrm{b}}$, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrow-width (lower-right) approximations w.r.t. NLO and WWb̄ predictions, respectively.

The transverse-momentum distribution of the harder b-jet is shown in Fig. 24 In the range below 200 GeV , which contains the bulk of the cross section, the NLO and finite-width corrections behave similarly as for the integrated cross section: LO predictions deviate from NLO ones by about $-20 \%$, and the error of the NWA ranges between +1 and $-4 \%$. Finite-width effects tend to increase with $p_{\mathrm{T}}$ and reach the $10 \%$ level around 300 GeV . Within the entire $p_{\mathrm{T}}$ range the LO/NLO ratios resulting from the $t \bar{t}$ and WWbb̄ calculations are almost equal. Equivalently, we find the same $\mathrm{d} \sigma_{\mathrm{tt}} / \mathrm{d} \sigma_{\mathrm{WWbb}}$ ratios in LO and NLO.


Fig. 25: Distribution in the transverse momentum of the b̄ di-jet system at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb百, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrow-width (lower-right) approximations w.r.t. NLO and WWb̄ predictions, respectively.

In Fig. 25 we show the transverse-momentum distribution of the $b \bar{b}$ di-jet system. This kinematic variable plays an important role in boosted-Higgs searches with a large t $\bar{t}$ background. In particular, the strategy proposed in Ref. [342] to extract a pp $\rightarrow \mathrm{H}(\rightarrow \mathrm{b} \overline{\mathrm{b}}) \mathrm{W}$ signal at the LHC is based on the selection of boosted $\mathrm{H} \rightarrow \mathrm{b} \overline{\mathrm{b}}$ candidates with $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}}>200 \mathrm{GeV}$, which permits to reduce $\mathrm{t} \overline{\mathrm{t}}$ contamination (and other backgrounds) in a very efficient way. As can be seen from Fig. 25, the suppression of $t \bar{t}$ production is indeed particularly strong at $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}} \gtrsim 150 \mathrm{GeV}$. This is due to kinematic constraints that characterise the LO and narrow-width approximations: in order to acquire $p_{\mathrm{T}, \mathrm{b}}>\left(m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2}\right) /\left(2 m_{\mathrm{t}}\right) \simeq 65 \mathrm{GeV}$ b-quarks need to be boosted via the $p_{\mathrm{T}}$ of their parent (anti)top quarks, and the fact that top and antitop quarks have opposite transverse momenta (at LO) makes it difficult to generate a b $\bar{b}$ system with high $p_{\mathrm{T}}$. The NLO and finite-width corrections undergo less stringent kinematic restrictions, resulting into a significant enhancement of $W W b \overline{\mathrm{~b}}$ events at large $p_{\mathrm{T}, \mathrm{b}}$. This is clearly reflected in the differences between the various curves in the left plot of Fig. 25. The most pronounced effect comes from the NLO corrections, where the $t \bar{t}$ system can acquire large transverse momentum by recoiling against extra jet radiation. As indicated by the right-upper plot, the NLO correction represents $50-80 \%$ of the cross section at high $p_{\mathrm{T}}$, corresponding to a huge $K$-factor of $2-5$. Finite-width effects (lower-right plot) lead to a further significant, although less dramatic, enhancement; for example, non-resonant topologies can lead to direct b $\overline{\mathrm{b}}$ production via high- $p_{\mathrm{T}}$ gluons that recoil against $\mathrm{W}^{+} \mathrm{W}^{-}$pairs. For $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}}>200 \mathrm{GeV}$, we find that $20-40 \%$ of the LO WWbb cross section is due to finite-width contributions, while this fraction decreases to $7-15 \%$ at NLO. This reduction is related to the dominance of the jet-emission contribution, which we expect to be rather well described by the NWA. On the other hand, an optimal suppression of the $t \bar{t}$ background will require a very tight jet-veto [342], and in this case we expect finite-width corrections to the NLO t̄ predictions to be as large as in LO.

The distribution in the missing transverse momentum, i.e. the vector sum of the $\nu_{e}$ and $\bar{\nu}_{\mu}$ trans-


Fig. 26: Distribution in the missing transverse momentum at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb $\overline{\mathrm{b}}$, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrowwidth (lower-right) approximations w.r.t. NLO and WWb̄̄ predictions, respectively.
verse momenta, is displayed in Fig. 26. This distribution is relevant for new-physics searches based on missing transverse energy plus jets and leptons. Its tail features a qualitatively similar behaviour as in the case of $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}}$, due to analogous kinematic constraints. However, in the case of $p_{\mathrm{T}, \mathrm{miss}}$ the corrections are less pronounced: the NLO correction does not exceed $40-50 \%$ of the full prediction, and finite-width contributions stay below roughly $10 \%$.

Figure 27 displays the distribution in the invariant mass of the positron and a b-jet, i.e. the visible products of a top-quark decay. More precisely, assuming that the charge of the b-jet is not known, the $\mathrm{e}^{+} \mathrm{b}$ pair is built by selecting the b-jet that yields the smallest invariant mass ${ }^{20}$ In narrow-width and LO approximation this kinematic quantity is characterised by a sharp upper bound, $M_{\mathrm{e}^{+} \mathrm{b}}^{2}<m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2} \simeq$ $(152 \mathrm{GeV})^{2}$, which renders it very sensitive to the top-quark mass. The value of $m_{\mathrm{t}}$ can be extracted with high precision using, for instance, the invariant-mass distribution of a positron and a $J / \psi$ from a $B$ meson decay [343, 338], an observable that is closely related to $M_{\mathrm{e}^{+} \mathrm{b}}$. In the region below the kinematic bound, the NLO corrections to $M_{\mathrm{e}^{+} \mathrm{b}}$ vary between $5-30 \%$, and the impact of the NLO shape distortion on a precision $m_{\mathrm{t}}$-measurement is certainly significant. For $M_{\mathrm{e}^{+} \mathrm{b}}<150 \mathrm{GeV}$, the NWA agrees with the WWb $\bar{b}$ predictions at the $1 \%$ level or better. In contrast, in the vicinity of the kinematic bound the impact of finite-width (and NLO) corrections becomes clearly more important, giving rise to a tail that extends above $M_{\mathrm{e}^{+} \mathrm{b}}^{2}=m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2}$. The resulting contribution to the total cross section is fairly small, but the impact of such finite-width effects on the top-mass measurement might be non-negligible, given the high $m_{\mathrm{t}}$-sensitivity of the $M_{\mathrm{e}^{+} \mathrm{b}}^{2} \simeq m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2}$ region.

[^130]

Fig. 27: Distribution in the invariant mass of the positron-b-jet system (as defined in the text) at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb $\bar{b}$, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrow-width (lower-right) approximations w.r.t. NLO and WWb $\bar{b}$ predictions, respectively.

### 10.4 CONCLUSIONS

Based on recent NLO QCD calculations, we have presented a systematic comparison of top-pair production and decay in narrow-top-width approximation, $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$, against the complete $\mathrm{pp} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$ process, which involves finite-top-width effects of non-resonant and off-shell type.

At the Tevatron and the LHC ( 7 and 14 TeV ), finite-top-width contributions to the integrated cross section (in the di-lepton channel) turn out not to exceed one percent. This confirms previous estimates based on the $\Gamma_{\mathrm{t}} \rightarrow 0$ extrapolation of $\mathrm{pp} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$ predictions. At the 7 TeV LHC, we also investigated differential observables that are relevant either for top-pair production as a signal or as a background in Higgs or new-physics searches. In the case of the b-jet transverse momentum and $p_{\mathrm{T}, \mathrm{miss}}$ distributions, finite-width effects remain very small over a large kinematic range and reach the $10 \%$ level only around 300 GeV . In contrast, the $p_{\mathrm{T}}$-distribution of the b $\overline{\mathrm{b}}$ di-jet system receives $\Gamma_{\mathrm{t}}$-corrections beyond 20-30\% for $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}} \gtrsim 200 \mathrm{GeV}$, a kinematic region that plays an important role in $\mathrm{pp} \rightarrow \mathrm{H}(\rightarrow \mathrm{b} \overline{\mathrm{b}}) \mathrm{W}$ searches based on boosted $\mathrm{H} \rightarrow \mathrm{b} \overline{\mathrm{b}}$ candidates. For the lepton-b-jet invariant-mass distribution-an observable that provides high sensitivity to the top-quark mass-finite-width corrections do not exceed one percent in the range that contains the bulk of the cross section, but become more sizable in the region of highest $m_{\mathrm{t}}$-sensitivity. This motivates more detailed studies of finite-width effects in the context of high-precision $m_{\mathrm{t}}$-measurements at the LHC. The results of this investigation of finite-width effects in t̄̄ production give also useful insights into possible limitations of treating associated top-pair production processes in the narrow-width approximation, since NLO calculations for $\mathrm{pp} \rightarrow \mathrm{WWb} \mathrm{\bar{b}}$ and similar reactions will not be available too soon.

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## 11. Strong and Smooth Ordering in Antenna Showers ${ }^{21}$


#### Abstract

We comment on strong and smooth ordering in antenna showers, and extend the definition of smooth ordering to include the case of $g \rightarrow q \bar{q}$ splittings. We define three observables in hadronic $Z$ decays that can be used to probe the subleading properties of shower models.


### 11.1 INTRODUCTION

Traditional parton showers are based on collinear factorization, and the shower evolution proceeds via $1 \rightarrow 2$ branchings, on which additional constraints have to be imposed to ensure momentum conservation and QCD coherence (see [344]). Antenna showers are instead based on momentum-conserving and intrinsically coherent $2 \rightarrow 3$ branchings, as pioneered by Ariadne [345, 346]. This note concerns the antenna shower implementation in the Vincia code [347], a plug-in to Pythia 8 [348], though we emphasize that the notion of smooth ordering could be applied to other shower types as well.

In leading-logarithmic (LL) antenna showers, the fundamental step is a Lorentz-invariant $2 \rightarrow 3$ branching process by which two on-shell "parent" partons are replaced by three on-shell "daughter" partons. This $2 \rightarrow 3$ process makes use of three ingredients [349]:

1. An antenna function that captures the leading tree-level singularities of QCD matrix elements.
2. An antenna phase space - an exact, momentum-conserving and Lorentz-invariant factorization of the pre- and post-branching phase spaces.
3. A kinematics map, specifying how the global orientation of the post-branching momenta are related to the pre-branching ones.
Antenna showers come in two varieties: global and sector. The two kinds differ in how the collinear singularities of gluons are partitioned among neighboring antennae, see [350, 351]. Here, we shall only be concerned with the global type [345, 352, 347, 349], in which the gluon-collinear singularity is partitioned such that two neigbouring antennae each contain "half" of it; their sum reproduces the full singularity.

If each antenna in a global shower is allowed to emit in its full phase space, the resulting shower evolution amounts to an incoherent addition of independently radiating dipoles. This tends to overcount regions in which several dipole terms contribute at the same level, i.e., in regions where dipole-dipole interference effects (or, equivalently, multipole effects) are important [353, 351]. The situation is analogous to, though less severe than, the case of traditional parton showers with virtuality-ordering [354], which represent an incoherent addition of independent monopoles. In parton/monopole showers, multiparton interference effects for soft radiation can be taken into account by the requirement of angular ordering [355], while in dipole/antenna showers, typically a measure of transverse momentum is used, such as

$$
\begin{equation*}
p_{\perp A}^{2}=\frac{s_{i j} s_{j k}}{s_{I K}} \tag{80}
\end{equation*}
$$

for a branching $I K \rightarrow i j k$, with $s_{a b} \equiv 2 p_{a} \cdot p_{b}=\left(p_{a}+p_{b}\right)^{2}$ for massless partons. Some alternative possibilities are compared in [349].

[^131]
### 11.2 STRONG AND SMOOTH ORDERING

In a strongly-ordered shower, each consecutive branching is required to occur at a lower scale in the evolution variable than that of the previous one: $Q_{n+1}<Q_{n}$. This can be represented as a step function in the evolution variable, multiplying the branching kernels. In a smoothly-ordered shower [349], the step function is replaced by a smooth dampening factor designed to leave the soft and collinear limits unchanged while suppressing radiation at scales above $\sim Q_{n}$. Specifically, for evolution in $p_{\perp}$, we replace the strong-ordering condition as follows,

$$
\begin{equation*}
\Theta\left(\hat{p}_{\perp}-p_{\perp}\right) P_{L L} \rightarrow P_{i m p} P_{L L} \equiv \frac{\hat{p}_{\perp}^{2}}{\hat{p}_{\perp}^{2}+p_{\perp}^{2}} P_{L L} \tag{81}
\end{equation*}
$$

where $\hat{p}_{\perp}$ characterizes the scale of the previous branching ${ }^{22}, p_{\perp}$ is the scale of the emission under consideration, and $P_{L L}$ is an ordinary LL shower kernel, which in our case is represented by a gluonemission antenna function. (We return to the case of $g \rightarrow q \bar{q}$ below.)

Thus, for $p_{\perp} \ll \hat{p}_{\perp}$ (the strongly-ordered limit) the smooth-ordering factor $P_{\text {imp }}$ tends to unity, while for $p_{\perp} \sim \hat{p}_{\perp}$ (the ordering threshold) it tends to $1 / 2$, and finally for $p_{\perp} \gg \hat{p}_{\perp}$ (highly unordered), it tends to zero $\propto \hat{p}_{\perp}^{2} / p_{\perp}^{2}$. Note that, since $P_{L L}$ is likewise $\propto 1 / p_{\perp}^{2}$, the net effect of the suppression factor is to modify the behavior of the splitting kernel from $1 / p_{\perp}^{2}$ in the strongly-ordered limits to $1 / p_{\perp}^{4}$ for highly unordered branchings, similar to what has been studied for initial-state parton showers in [356]; above the strong-ordering threshold, the branching probability is explicitly suppressed beyond LL.

For a rigourous interpretation of the $P_{\text {imp }}$ factor one would have to analyze the $2 \rightarrow 4$ antennae [79] and check that the combination of two $2 \rightarrow 3$ antennae times this factor does indeed reproduce subleading aspects of the full $2 \rightarrow 4$ function. In the absence of such a study, one may still physically interpret its purpose in the following way: the LL antenna functions are derived assuming the outgoing partons/jets to be massless. This is a good approximation if the virtuality that they can acquire (through further showering) is restricted by the strong-ordering threshold. When allowing unordered branchings, however, the corresponding Feynman diagrams contain highly off-shell propagators, which the $P_{\text {imp }}$ factor attempts to mimic by introducing an "effective mass" in the denominator of eq. 81.

For gluon emissions, it was shown in [349] that the smooth-ordering condition does lead to a systematic improvement in the shower. Since it simultaneously guarantees a complete phase-space coverage (contrary to the case for strong ordering [357, 349]), it is the default option in Vincia.

Antenna showers including $g \rightarrow q \bar{q}$ splittings were studied in [358], in which evolution in $m_{q \bar{q}}^{2}$ was introduced for such branchings. This is based on the observation [359] that the scale controlling the divergences of $g \rightarrow q \bar{q}$ splittings is the invariant mass of the pair, not its $p_{\perp}$. By analogy with the physical interpretation given to the $P_{\text {imp }}$ factor for gluon emissions above, it therefore seems well-motivated to study a "generalized" $P_{\text {imp }}$ factor where each scale depends on whether we are dealing with a gluon or a quark:

$$
\begin{equation*}
P_{i m p}=\frac{\hat{Q}_{E}^{2}}{\hat{Q}_{E}^{2}+Q_{E}^{2}}, \tag{82}
\end{equation*}
$$

where $Q_{E}$ is the evolution variable: $p_{\perp}$ for gluons and invariant mass for quark-antiquark pairs.
We can assess the improvement that this produces in the shower by plotting the ratio of the shower approximation vs. the LO matrix element for $Z \rightarrow q \bar{q}^{\prime} q^{\prime} \bar{q}$ and $Z \rightarrow q \bar{q}^{\prime} q^{\prime} g \bar{q}$. This is shown in fig. 28, where the histograms represent the distribution of $\log _{10}(\mathrm{PS} / \mathrm{ME})$ in a flat phase-space scan, normalized to unity (i.e., the same type of distributions that were shown in [349, 358, 351]). Points to the left of zero are undercounted by the shower approximation, while points to the right are overcounted. Although the agreement is by no means perfect, we do observe a slight improvement in the shower approximation

[^132]

Fig. 28: Comparison between generalized $\tilde{P}_{i m p}$ and "old" $P_{i m p}$ factor in the global shower approximations to LO matrix elements, for processes involving a $g \rightarrow q \bar{q}$ splitting. Left: $Z \rightarrow q \bar{q}^{\prime} q^{\prime} \bar{q}$. Right: $Z \rightarrow q \bar{q}^{\prime} q^{\prime} q \bar{q}$. In both cases, GKS matching to the LO matrix element for the preceding multiplicity ( $Z \rightarrow 3$ and $Z \rightarrow 4$, respectively) has been included, and the Ariadne factor was applied to $g \rightarrow q \bar{q}$ splittings.
when the $P_{i m p}$ factor is defined in terms of $Q_{E}$ (solid black histogram), as compared to the definition used previously (dashed histogram). Note that we used the so-called Ariadne factor in the shower approximation for all cases, see [358], and that the distributions were made including GKS matching to the preceding multiplicities [349].

### 11.3 SENSITIVE OBSERVABLES IN HADRONIC Z DECAYS

The properties of shower and matrix-element matching algorithms are coming under increasing scrutiny, not least due to the desire of achieving reliable descriptions of jet production and jet properties, such as jet substructure, for signal and background estimates at the LHC.

For final-state radiation, i.e., jet broadening and jet splitting, hadronic $Z$ decays are the main reference, with a large set of events shapes and jet resolutions/rates being used to constrain and tune shower algorithms (see, e.g., [360, 344]). However, in the logarithmically dominated regions, these observables are typically dominated by leading logs, and are well described by all coherent and reasonably well-tuned shower algorithms on the market. In order to probe the subleading properties in a more dedicated way, we have found the following three simple observables useful, each designed to isolate a specific aspect.

We consider hadronic $Z$ events (photon ISR is switched off, and matching beyond 3 jets is switched off for the strongly-ordered showers) and use the $k_{T}$ clustering algorithm [361] to cluster all events back to two jets. The $3 \rightarrow 2$ clustering scale is denoted $y_{23}=k_{T 3}^{2} / m_{Z}^{2}$, and so on for higher jet numbers. We require all $y_{i j}$ entering in the observables below to be greater than 0.005 , to remove contamination from $B$ decays and lower scales. Since the original topology contains two jets, we also keep track of which "side" each clustering happens on. Strong ordering corresponds to $y_{23} \gg y_{34} \gg \ldots$, while events with, e.g., $y_{34} \sim y_{23}$ should be more sensitive to the ordering condition and to the effective $1 \rightarrow 3$ spliting kernels.

The first observable is thus simply the ratio $y_{34} / y_{23}$, in events where the $4 \rightarrow 3$ and $3 \rightarrow 2$ clusterings happen in the same jet. This distribution is illustrated in the left-hand pane of fig. 29, with logarithmic axes. Vertical error bars indicate the expected $1 \sigma$ statistical error with 400 k hadronic $Z$ decays. Since the $k_{T}$ algorithm allows for unordered clustering scales, the distribution extends beyond $\xi_{24}=\ln \left(y_{34} / y_{24}\right)=0$. Default Pythia (thick solid line) is compared to three different Vincia settings: smooth (thin solid) and strong (dashed) ordering in $p_{\perp}$ and strong ordering in dipole virtuality, $m_{D}$ (dotted). Note here that ordering in the variables $p_{\perp}$ or $m_{D}$ does not directly imply ordering in $k_{T}$.


Fig. 29: Left: $\xi_{24}=\ln \left(y_{34} / y_{23}\right)$ in "same-side" 4-jet events. Right: Ratio of jet masses, $m_{L}^{2} / m_{H}^{2}$, in "compressed" 4-jet events. Error bars indicate expected $1 \sigma$ statistical errors with 400 k hadronic $Z$ decays.

The fact that the $P_{\text {imp }}$ factor also suppresses branchings slightly below the strong-ordering threshold is manifest in the thin solid line lying below the other ones in the region just below zero, which should be statistically significant with a sample size of $\sim 0.5 \mathrm{M}$ events. Note as well that these distributions become indistinguishable if one does not make the requirement of sameside clustering (not shown), presumably since opposite-side collinear splittings then dominate.

A related observable is shown in the right-hand pane of fig. 29. To force a "compressed" scale hierarchy, we impose the cut $y_{34}>0.5 y_{23}$, and plot the ratio $M_{L}^{2} / M_{H}^{2}$ of the masses of the jets at the end of the clustering. With four partons at LO, the light jet mass is zero if both the $4 \rightarrow 3$ and $3 \rightarrow 2$ clusterings happen in the same jet, while it is non-zero otherwise. Thus, the region close to zero isolates events with a $1 \rightarrow 3$ splitting occurring in one of the jets, while the region above $\sim 0.25$ is dominated by opposite-side $1 \rightarrow 2$ splittings. In Pythia and in mass-ordered Vincia, the peak at zero is stronger than in the $p_{\perp}$-ordered Vincia cases, while there is no difference between strong and smooth ordering in this variable. It thus serves as a useful complement to $\xi_{24}$.

Finally, in fig. 30, we consider 4-jet events in which the second and third jets (ordered in energy) are nearly collinear and back-to-back to the hardest jet. Specifically, we impose the cuts $\theta_{12}>120^{\circ}$, $\theta_{13}>120^{\circ}$, and $\theta_{23}<30^{\circ}$. We then plot the angle of the fourth (softest) jet with respect to the hardest one. Again the strong and smooth ordering options are indistinguishable, but interesting differences with respect to both Pythia and mass-ordered Vincia are visible. Mass-ordering tends to produce a broader distribution, with more radiation at right angles to the hardest jet (consistent with mass-ordering prioritizing wide-angle emissions over collinear ones), and the $p_{\perp}$-ordered Vincia showers exhibit a stronger collinear peak than the Pythia one. A similar observable was proposed in [362].

We conclude that, if all three observables could be measured with an accuracy of $\sim 5-10 \%$ or better, a useful and multi-dimensional constraint on the subleading shower aspects would be obtained, including sensitivity both to the type and shape of the ordering condition, and to the form of the effective $1 \rightarrow 3$ probabilities produced by the shower. We emphasize that we have here restricted our attention to shower models that are virtually indistinguishable on all other observables we have considered.

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Fig. 30: Angle between the hardest $\left(1^{\text {st }}\right)$ and softest $\left(4^{\text {th }}\right)$ jets in "collinear" 4 -jet events. Error bars indicate expected $1 \sigma$ statistical errors with 400 k hadronic $Z$ decays.
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## 12. PERTURBATIVE UNCERTAINTIES AND RESUMMATION FOR EXCLUSIVE JET CROSS SECTIONS ${ }^{23}$

### 12.1 Introduction

In this writeup we discuss predictions for exclusive jet cross sections, which have a particular number of jets in the final state. There are several motivations for analyzing events by dividing the data into exclusive jet bins, in particular when the relevant backgrounds strongly depend on the number of jets, or when the sensitivity can be increased by optimizing the analysis for the individual jet bins. As our primary example we will consider the Higgs analysis in the $H \rightarrow W W$ channel, which is performed separately in exclusive 0 -jet, 1 -jet, and 2 -jet bins [363, 364, 365]. Other examples are vector-boson fusion analyses, which are typically performed in the exclusive 2-jet channel, boosted $H \rightarrow b \bar{b}$ analyses that include a veto on additional jets, as well as $H \rightarrow \tau \tau$ and $H \rightarrow \gamma \gamma$ which benefit from improved sensitivity when the Higgs recoils against a jet. The importance of the Higgs +1 jet channel in $H \rightarrow \tau \tau$ and $H \rightarrow W W^{*}$ was demonstrated explicitly in Refs. [366, 367]. Another motivation for studying exclusive jet bins are the $W+$ jets channels, which are important backgrounds for new physics searches. We will use the notation $\sigma_{N}$ for an exclusive $N$-jet cross section (with exactly $N$ jets), and the notation $\sigma_{\geq N}$ for an inclusive $N$-jet cross section (with $N$ or more jets).

To explore the implications of the jet bin restrictions, consider a simple example where we divide the total cross section, $\sigma_{\text {total }}$, into an exclusive 0 -jet bin, $\sigma_{0}\left(p^{\mathrm{cut}}\right)$, and the remaining inclusive $(\geq 1)$-jet bin, $\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right)$,

$$
\begin{equation*}
\sigma_{\mathrm{total}}=\int_{0}^{p^{\mathrm{cut}}} d p \frac{d \sigma}{d p}+\int_{p^{\mathrm{cut}}} d p \frac{d \sigma}{d p} \equiv \sigma_{0}\left(p^{\mathrm{cut}}\right)+\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right) . \tag{83}
\end{equation*}
$$

Here $p$ denotes the kinematic variable which is used to divide up the cross section into jet bins. A typical choice is $p \equiv p_{T}^{\text {jet }}$, defined by the largest $p_{T}$ of any jet in the event, such that $\sigma_{0}\left(p_{T}^{\text {cut }}\right)$ only contains events with jets having $p_{T} \leq p_{T}^{\mathrm{cut}}$, and $\sigma_{\geq 1}\left(p_{T}^{\mathrm{cut}}\right)$ contains events with at least one jet with $p_{T} \geq p_{T}^{\text {cut }}$. By defining $\sigma_{0}\left(p_{T}^{\text {cut }}\right)$ and $\sigma_{\geq 1}\left(p_{T}^{\text {cut }}\right)$ one has divided up initial-state radiation from the

[^133]colliding hard partons and soft radiation in the event. This restriction on additional emissions changes the coefficients appearing in the $\alpha_{s}$ expansion and leads to the appearance of double and single logarithms of the form $\alpha_{s} \ln ^{2}\left(p^{\text {cut }} / Q\right)$ and $\alpha_{s} \ln \left(p^{\text {cut }} / Q\right)$ (with higher powers $\alpha_{s}^{n} \ln ^{m \leq 2 n}\left(p^{\text {cut }} / Q\right)$ appearing at higher orders in perturbation theory). Here $Q$ is the hard scale of the process, such as $Q=m_{H}$ for Higgs production, and most often we have $p^{\text {cut }} \ll Q$. These changes to the perturbation series can modify the convergence of fixed-order results and make it prudent to consider resummed cross section predictions that include an all-orders resummation of the large logarithms. For $N$ jets the analog of Eq. 833) is $\sigma_{\geq N}=\sigma_{N}\left(p_{N+1}^{\mathrm{cut}}\right)+\sigma_{\geq N+1}\left(p_{N+1}^{\mathrm{cut}}\right)$ and the same discussion applies regarding the large logarithms of $p_{N}^{\text {cut }}$ that are not present in $\sigma_{\geq N}$, but are present in each of $\sigma_{N}$ and $\sigma_{\geq N+1}$.

The definition of $\sigma_{0}\left(p^{\mathrm{cut}}\right)$ may include dependence on rapidity and on the grouping of particles. For a jet-based variable like $p_{T}^{\text {jet }}$ the former is induced by only considering jets within the rapidity range $\left|\eta^{\text {jet }}\right| \leq \eta^{\text {cut }}$, and the latter enters through the choice of jet algorithm. These dependencies make theoretical predictions more difficult. In Higgs production via gluon fusion the cross section is known to next-to-next-to-leading order (NNLO) [208, 368, 207, 209, 210, 211, 369, 370], and NNLO results including full kinematic information are available through FeHiP [214, 371] and HNNLO [90, 216] (as well as by combining the total NNLO cross section with MCFM [157, 372] for some distributions). When the measurements are performed in exclusive jet bins, the perturbative uncertainties in the theoretical predictions must also be evaluated separately for each individual jet bin [373]. When combining channels with different jet multiplicities, the correlations between the theoretical uncertainties can be significant and must be taken into account [26]. The perturbative predictions can be made more precise by including a resummation of large $p^{\text {cut }}$ dependent logarithms on top of the fixed-order predictions. At the leading logarithmic level this can be achieved with standard parton shower Monte Carlo programs, regardless of the precise definition of $p^{\mathrm{cut}}$. So far a next-to-next-to-leading logarithmic (NNLL) resummed result for a jet-veto variable only exists for beam thrust [374], $\mathcal{T}_{\mathrm{cm}}$, which is a rapidity weighted $E_{T}$-like inclusive variable. The definitions of the jet-veto variables we will use are

$$
\begin{equation*}
p_{T}^{\text {jet }}=\left|\sum_{k \in \mathrm{jet}} \vec{p}_{T k}\right|, \quad \quad \mathcal{T}_{\mathrm{cm}}=\sum_{k}\left|\vec{p}_{T k}\right| e^{-\left|\eta_{k}\right|}=\sum_{k}\left(E_{k}-\left|p_{k}^{z}\right|\right) . \tag{84}
\end{equation*}
$$

For $p_{T}^{\text {jet }}$ our jets are defined using anti- $k_{T}$ [341] with $R=0.5$, and we consider jets that satisfy a rapidity cut $|\eta| \leq \eta^{\text {cut }}$. For $\mathcal{T}_{\text {cm }}$ the sum is over all objects in the final state except the Higgs decay products, and can in principle be considered over particles, topo-clusters, or jets with a small $R$ parameter. In all our results we consistently use MSTW2008 NNLO PDFs [262].

In this writeup we will explore fixed NNLO and resummed NNLL+NNLO predictions for $H+$ 0 -jet cross sections and compare various methods for evaluating the uncertainty as a function of cuts on $p_{T}^{\text {jet }}$ and $\mathcal{T}_{\mathrm{cm}}$. The three methods we will discuss for evaluating the uncertainties in exclusive jet cross sections are
A) "Direct Exclusive Scale Variation". Here the uncertainties are evaluated by directly varying the renormalization and factorization scales in the fixed-order predictions for each exclusive jet cross section $\sigma_{N}$. This implies that the uncertainties are $100 \%$ correlated for different $N$ s.
B) "Combined Inclusive Scale Variation", as proposed in Ref. [26] and utilized in Refs. [363, 364 365]. Here, the perturbative uncertainties in the inclusive $N$-jet cross sections, $\sigma_{\geq N}$, are treated as the primary uncertainties that can be evaluated by scale variations in fixed-order perturbation theory. These uncertainties are treated as uncorrelated for different $N$. The exclusive $N$-jet cross sections are obtained using $\sigma_{N}=\sigma_{\geq N}-\sigma_{\geq N+1}$. The uncertainties and correlations follow from standard error propagation, including the appropriate anticorrelations between $\sigma_{N}$ and $\sigma_{N \pm 1}$ related to the division into jet bins.
C) "Uncertainties from Resummation." Resummed calculations for exclusive jet cross sections can provide uncertainty estimates that allow one to simultaneously include both types of correlated
and anticorrelated uncertainties as in methods A and B. The magnitude of the uncertainties may also be reduced from the resummation of large logarithms.
In all three methods, adding the exclusive jet cross sections yields the expected scale variation in the total cross section. Method B avoids a potential underestimate of the uncertainties in individual jet bins due to strong cancellations that can potentially take place in method A. Method B produces realistic perturbative uncertainties for exclusive jet cross sections when using fixed-order predictions for various processes, since it accounts for the presence of large logarithms at higher orders caused by the jet binning. In Method C one utilizes higher-order resummed predictions for the exclusive jet cross sections, which allow one to obtain improved central values and further refined uncertainty estimates.

The basic structure of the large logarithms in the perturbative series is discussed in Sec. 12.2. In Sec. 12.3 we discuss and compare the above three methods to determine the perturbative uncertainties. The work discussed here regarding methods A, B, and C builds on work done in Refs. [375, 26], was initiated at Les Houches, and has also been incorporated in the second Higgs Yellow Book report [376] (Secs. 5.2 and 5.5.) We also review recent work by others that can be found in [376](Sec. 5.3).

Note that here we are only discussing the theoretical uncertainties due to unknown higher-order perturbative corrections, which are commonly estimated using scale variation. Parametric uncertainties, such as PDF choices and $\alpha_{s}\left(m_{Z}\right)$ uncertainties, must be treated appropriately as common sources for all investigated channels.

### 12.2 Theoretical Motivation

### 12.21 Structure of the Perturbative Series

We begin by discussing the structure of the large logarithms in exclusive jet cross sections. For Higgs production from gluon fusion with $p_{T}^{\text {jet }} \leq p_{T}^{\text {cut }}$ the leading double logarithms appearing at $\mathcal{O}\left(\alpha_{s}\right)$ are

$$
\begin{equation*}
\sigma_{0}\left(p_{T}^{\mathrm{cut}}\right)=\sigma_{B}\left(1-\frac{3 \alpha_{s}}{\pi} 2 \ln ^{2} \frac{p_{T}^{\mathrm{cut}}}{m_{H}}+\cdots\right), \tag{85}
\end{equation*}
$$

where $\sigma_{B}$ is the Born (tree-level) cross section.
The total cross section only depends on the hard scale $Q=m_{H}$, which means by choosing the factorization and renormalization scales $\mu_{f} \simeq \mu_{r} \simeq m_{H}$, the fixed-order expansion does not contain large logarithms and has the structure

$$
\begin{equation*}
\sigma_{\text {total }} \simeq \sigma_{B}\left[1+\alpha_{s}+\alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] . \tag{86}
\end{equation*}
$$

Our expressions for perturbative series such as this one are schematic, showing the scaling of the terms without the coefficient functions. The convolution with the parton distribution functions (PDFs) are also not displayed. For $g g \rightarrow H$, the coefficients of this series can be large, corresponding to the well-known large K factors. As usual, varying the scale in $\alpha_{s}(\mu)$ (and the PDFs) one obtains an estimate of the size of the missing higher-order terms in this series, which we denote by $\Delta_{\text {total }}$.

The inclusive 1 -jet cross section has the perturbative structure

$$
\begin{equation*}
\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right) \simeq \sigma_{B}\left[\alpha_{s}\left(L^{2}+L+1\right)+\alpha_{s}^{2}\left(L^{4}+L^{3}+L^{2}+L+1\right)+\mathcal{O}\left(\alpha_{s}^{3} L^{6}\right)\right], \tag{87}
\end{equation*}
$$

where the logarithms $L=\ln \left(p^{\text {cut }} / m_{H}\right)$. For $p^{\text {cut }} \ll m_{H}$ these logarithms can get large enough to overcome the $\alpha_{s}$ suppression. In the limit $\alpha_{s} L^{2} \simeq 1$, the fixed-order perturbative expansion breaks down and the logarithmic terms must be resummed to all orders in $\alpha_{s}$ to obtain a meaningful result. For typical experimental values of $p^{\text {cut }}$ fixed-order perturbation theory can still be considered, but the logarithms cause large corrections at each order and dominate the series.

The exclusive 0 -jet cross section is equal to the difference between Eqs. (86) and (87), and so has the schematic structure
$\sigma_{0}\left(p^{\mathrm{cut}}\right)=\sigma_{\text {total }}-\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right)$

$$
\begin{equation*}
\simeq \sigma_{B}\left\{\left[1+\alpha_{s}+\alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right]-\left[\alpha_{s}\left(L^{2}+L+1\right)+\alpha_{s}^{2}\left(L^{4}+L^{3}+L^{2}+L+1\right)+\mathcal{O}\left(\alpha_{s}^{3} L^{6}\right)\right]\right\} \tag{88}
\end{equation*}
$$

In this difference, the large positive corrections in $\sigma_{\text {total }}$ partly cancel against the large negative logarithmic corrections in $\sigma_{\geq 1}$. For example, at $\mathcal{O}\left(\alpha_{s}\right)$ there is a value of $L$ for which the $\alpha_{s}$ terms in Eq. (88) cancel exactly. At this $p^{\text {cut }}$ the NLO 0 -jet cross section has vanishing scale dependence and is equal to the LO cross section, $\sigma_{0}\left(p^{\mathrm{cut}}\right)=\sigma_{B}$. Due to this cancellation, a standard use of scale variation in $\sigma_{0}\left(p^{\mathrm{cut}}\right)$ does not actually probe the size of the large logarithms, and does not provide an estimate of $\Delta_{\text {cut }}$. This issue impacts the uncertainties in the experimentally relevant region for $p^{\text {cut }}$.

For example, for $g g \rightarrow H$ (with $\sqrt{s}=7 \mathrm{TeV}, m_{H}=165 \mathrm{GeV}, \mu_{f}=\mu_{r}=m_{H} / 2$ ), one finds [214, 371, 90, 216]

$$
\begin{align*}
\sigma_{\text {total }} & =(3.32 \mathrm{pb})\left[1+9.5 \alpha_{s}+35 \alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] \\
\sigma_{\geq 1}\left(p_{T}^{\mathrm{jet}} \geq 30 \mathrm{GeV},\left|\eta^{\mathrm{jet}}\right| \leq 3.0\right) & =(3.32 \mathrm{pb})\left[4.7 \alpha_{s}+26 \alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] \tag{89}
\end{align*}
$$

In $\sigma_{\text {total }}$ one can see the impact of the well-known large $K$ factors. (Using instead $\mu_{f}=\mu_{r}=m_{H}$ the $9.5 \alpha_{s}$ and $35 \alpha_{s}^{2}$ coefficients in $\sigma_{\text {total }}$ increase to $11 \alpha_{s}$ and $65 \alpha_{s}^{2}$.) In $\sigma \geq 1$, one can see the impact of the large logarithms on the perturbative series. Taking their difference to get $\sigma_{0}$, one observes a sizeable numerical cancellation between the two series at each order in $\alpha_{s}$.

### 12.22 Perturbative Series for the Event Fraction

Experimentally the desired quantity which incorporates the jet-veto cut is the exclusive 0-jet event fraction

$$
\begin{equation*}
f_{0}\left(p^{\mathrm{cut}}\right)=\frac{\sigma_{0}\left(p^{\mathrm{cut}}\right)}{\sigma_{\mathrm{total}}}=1-\frac{\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right)}{\sigma_{\mathrm{total}}} . \tag{90}
\end{equation*}
$$

One option for treating $f_{0}\left(p^{\mathrm{cut}}\right)$ is to consider it as a derived quantity, given the basic observables $\left\{\sigma_{0}, \sigma_{\text {total }}\right\}$ or $\left\{\sigma_{\geq 1}, \sigma_{\text {total }}\right\}$. In this approach, which was utilized in Ref. [26] and Ref. [376](Secs. 5.2 and 5.5), one propagates the uncertainties from the $\sigma_{i} \mathrm{~s}$ to derive those for $f_{0}\left(p^{\mathrm{cut}}\right)$. This approach is natural from the perspective of utilizing log-resummed computations for $\sigma_{0}\left(p^{\mathrm{cut}}\right)$. In particular, it maintains the constraint that for large $p^{\text {cut }}$ we have monotonic convergence of $\sigma_{0} \rightarrow \sigma_{\text {total }}$ and $f_{0} \rightarrow 1$, a property that relies on a phase space cut reducing the cross section, but does not depend on perturbation theory.

When using fixed-order predictions for the various cross sections, an alternative to Eq. (90) considered in Ref. [376](Sec. 5.3) is to analyze the perturbation theory for $f_{0}\left(p^{\mathrm{cut}}\right)$ directly. In this case different schemes of organizing the perturbation series, by keeping or dropping various $\mathcal{O}\left(\alpha_{s}^{3}\right)$ terms, give a method to estimate the size of the higher-order perturbative corrections. Three such schemes were considered in Ref. [376](Sec. 5.3) (which we label here by schemes 1,2,3). It is convenient to define the perturbative corrections to the cross section by dividing each of them by the Born cross section $\sigma_{B}$, such that we can write

$$
\begin{align*}
\sigma_{\text {total }} & =\sigma_{B}\left[1+\hat{\sigma}_{\text {total }}^{(1)}+\hat{\sigma}_{\text {total }}^{(2)}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right], \\
\sigma_{\geq 1}\left(p^{\text {cut }}\right) & =\sigma_{B}\left[\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\text {cut }}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\text {cut }}\right)+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] . \tag{91}
\end{align*}
$$

With this notation the result of treating $f_{0}$ as a derived quantity is

$$
\begin{equation*}
\left[f_{0}\left(p^{\mathrm{cut}}\right)\right]^{(\text {scheme } 1)}=1-\frac{\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\mathrm{cut}}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\mathrm{cut}}\right)}{1+\hat{\sigma}_{\text {total }}^{(1)}+\hat{\sigma}_{\text {total }}^{(2)}}+\mathcal{O}\left(\alpha_{s}^{3}\right), \tag{92}
\end{equation*}
$$

while at the same order in perturbation theory we can also consider the following expressions for $f_{0}$ :

$$
\begin{align*}
& {\left[f_{0}\left(p^{\mathrm{cut}}\right)\right]^{\text {(scheme } 2)}=1-\frac{\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\mathrm{cut}}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\mathrm{cut}}\right)}{1+\hat{\sigma}_{\text {total }}^{(1)}}+\mathcal{O}\left(\alpha_{s}^{3}\right),} \\
& {\left[f_{0}\left(p^{\mathrm{cut}}\right)\right]^{(\text {scheme } 3)}=1-\left[\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\mathrm{cut}}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\mathrm{cut}}\right)\right]+\hat{\sigma}_{\geq 1}^{(1)} \hat{\sigma}_{\text {total }}^{(1)}+\mathcal{O}\left(\alpha_{s}^{3}\right) .} \tag{93}
\end{align*}
$$

We will contrast using the expressions in Eq. (92) and Eq. (93) with various methods for analyzing the uncertainty in our discussion below.

### 12.3 Uncertainty Analysis for Exclusive Jet Bins

As described in Sec. 12.21, the phase space restriction defining $\sigma_{0}$ changes its perturbative structure compared to that of $\sigma_{\text {total }}$. In general this gives rise to an additional perturbative uncertainty due to missing higher-order terms depending on $p^{\text {cut }}$. We will call the associated jet-binning uncertainty $\Delta_{\text {cut }}$. This can be thought of as an uncertainty related to the presence of large logarithms of $p^{\text {cut }}$ at higher orders in perturbation theory. In Eq. (83) both $\sigma_{0}$ and $\sigma_{\geq 1}$ depend on the phase space cut, $p^{\text {cut }}$, and by construction this dependence cancels in $\sigma_{0}+\sigma_{\geq 1}$. Hence, the additional uncertainty $\Delta_{\text {cut }}$ induced by $p^{\text {cut }}$ must be $100 \%$ anticorrelated between $\sigma_{0}\left(p^{\text {cut }}\right)$ and $\sigma_{\geq 1}\left(p^{\text {cut }}\right)$, such that it cancels in their sum. For example, using a covariance matrix to model the uncertainties and correlations, the contribution of $\Delta_{\text {cut }}$ to the covariance matrix for $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ must be of the form

$$
C_{\mathrm{cut}}=\left(\begin{array}{cc}
\Delta_{\mathrm{cut}}^{2} & -\Delta_{\mathrm{cut}}^{2}  \tag{94}\\
-\Delta_{\mathrm{cut}}^{2} & \Delta_{\mathrm{cut}}^{2}
\end{array}\right) .
$$

The questions then are: (1) How can we estimate $\Delta_{\text {cut }}$ in a simple way, and (2) how is the perturbative uncertainty $\Delta_{\text {total }}$ of $\sigma_{\text {total }}$ related to the uncertainties of $\sigma_{0}$ and $\sigma_{\geq 1}$ ?

### 12.31 Perturbative Uncertainties for Method A

When using method A to estimate the perturbative uncertainties one simply uses a common scale variation to estimate the uncertainty $\Delta_{0}$ in $\sigma_{0}$ and the uncertainty $\Delta_{\geq 1}$ in $\sigma_{\geq 1}$. By doing so the uncertainties are $100 \%$ correlated, corresponding to a covariance matrix in method A for $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ given by

$$
C_{A}=\left(\begin{array}{cc}
\Delta_{0}^{2} & \Delta_{0} \Delta_{\geq 1}  \tag{95}\\
\Delta_{0} \Delta_{\geq 1} & \Delta_{\geq 1}^{2}
\end{array}\right)
$$

Here $\Delta_{\text {total }}=\Delta_{0}+\Delta_{\geq 1}$ is the scale uncertainty in $\sigma_{\text {total }}$. When instead of $\sigma_{0}$ we directly calculate the 0 -jet event fraction $f_{0}$ using Eq. (92) or one of the expressions in Eq. (93), we can again determine the method A uncertainty estimate by scale variation in $f_{0}$ (we will refer to these results as methods $A_{1}, A_{2}$, and $A_{3}$ respectively).

In this method $\Delta_{\text {cut }}$ is not included because, as explained below Eq. (88), varying the perturbative scale in $\Delta_{0}$ does not probe the presence of the higher order large logarithms depending on $p^{\text {cut }}$. This method can lead to an underestimate of the perturbative uncertainty in $\sigma_{0}$ (and hence $f_{0}$ ), since there is a region of $p^{\text {cut }}$ values where scale variation is no longer a reasonable estimate of higher order corrections because of the vanishing of the $\mu$ dependence.

### 12.32 Perturbative Uncertainties for Method B

Since the perturbative series for $\sigma_{\geq 1}$ in Eq. (87) is dominated by the large logarithms of $p^{\text {cut }}$, we can use its scale variation $\Delta_{\geq 1}$ to get an estimate for their size by taking $\Delta_{\text {cut }}=\Delta_{\geq 1}$ [26]. Since $\Delta_{\text {cut }}$ and $\Delta_{\text {total }}$ are by definition uncorrelated, by setting $\Delta_{\text {cut }}=\Delta_{\geq 1}$ we are effectively treating the perturbative
series for $\sigma_{\text {total }}$ and $\sigma_{\geq 1}$ as independent with uncorrelated perturbative uncertainties. That is, considering $\left\{\sigma_{\text {total }}, \sigma_{\geq 1}\right\}$, the covariance matrix is diagonal,

$$
\left(\begin{array}{cc}
\Delta_{\text {total }}^{2} & 0  \tag{96}\\
0 & \Delta_{\geq 1}^{2}
\end{array}\right)
$$

where $\Delta_{\text {total }}$ and $\Delta_{\geq 1}$ are evaluated by separate scale variations in the fixed-order predictions for $\sigma_{\text {total }}$ and $\sigma_{\geq 1}$. This is consistent, since for small $p^{\text {cut }}$ the two series have very different structures. In particular, there is no reason to believe that the same cancellations in $\sigma_{0}$ will persist at every order in perturbation theory at a given $p^{\text {cut }}$. It follows that the perturbative uncertainty in $\sigma_{0}=\sigma_{\text {total }}-\sigma_{\geq 1}$ is given by $\Delta_{\text {total }}^{2}+\Delta_{\geq 1}^{2}$, and the resulting covariance matrix for $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ in method B is

$$
C_{B}=\left(\begin{array}{cc}
\Delta_{\geq 1}^{2}+\Delta_{\text {total }}^{2} & -\Delta_{\geq 1}^{2}  \tag{97}\\
-\Delta_{\geq 1}^{2} & \Delta_{\geq 1}^{2}
\end{array}\right) .
$$

Note that all of $\Delta_{\text {total }}$ occurs in the uncertainty for $\sigma_{0}$. This is reasonable from the point of view that $\sigma_{0}$ starts at the same order in $\alpha_{s}$ as $\sigma_{\text {total }}$ and contains the same leading virtual corrections. The method B uncertainty for the event fraction $f_{0}$ follows most naturally by error propagation from the cross sections, treating it as a derived quantity.

The limit $\Delta_{\text {cut }}=\Delta_{\geq 1}$ that Eq. (97) is based on is of course an approximation. However, the preceding arguments show that it is a more reasonable starting point than method A , since the latter does not account for the additional $p^{\text {cut }}$ induced uncertainties.

The generalization of the above discussion to more jets and several jet bins is straightforward. For the $N$-jet bin we replace $\sigma_{\text {total }} \rightarrow \sigma_{\geq N}, \sigma_{0} \rightarrow \sigma_{N}$, and $\sigma_{\geq 1} \rightarrow \sigma_{\geq N+1}$. If the perturbative series for $\sigma_{\geq N}$ exhibits large $\alpha_{s}$ corrections due to its logarithmic series or otherwise, then the presence of a different series of large logarithms in $\sigma_{\geq N+1}$ will again lead to cancellations when we consider the difference $\sigma_{N}=\sigma_{\geq N}-\sigma_{\geq N+1}$. These two cross sections will have different series for their double logarithms since the number of active partons and their color structure differ. In this situation $\Delta_{\geq N+1}$ will again give a better estimate for the extra $\Delta_{\text {cut }}$ type uncertainty that arises from separating $\sigma_{\geq N}$ into $\sigma_{N}$ and $\sigma_{\geq N+1}$.

### 12.33 Perturbative Uncertainties for Method C

In method C we assess the perturbative uncertainties using resummed predictions for variables $p^{\text {cut }}$ that implement a jet veto, following Refs. [375, 26]. An advantage of using resummed predictions is that they contain perturbation theory scale parameters which allow for an evaluation of two components of the theory error, one which is $100 \%$ correlated with the total cross section (as in method A), and one related to the presence of the jet-bin cut which is anti-correlated between neighboring jet bins (as in method B).

The resummed $H+0$-jet cross section predictions of Ref. [375] follow from a factorization theorem for the 0 -jet cross section [374], $\sigma_{0}\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)=H \mathcal{I}_{g i} \mathcal{I}_{g j} \otimes S f_{i} f_{j}$, where $H$ contains hard virtual effects, the $\mathcal{I}_{\text {s }}$ and $S$ describe the veto-restricted collinear and soft radiation, and the $f$ s are standard parton distributions. Fixed-order perturbation theory is carried out at three scales, a hard scale $\mu_{H}^{2} \sim m_{H}^{2}$ in $H$, and beam and soft scales $\mu_{B}^{2} \sim m_{H} \mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$ and $\mu_{S}^{2} \sim\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)^{2}$ for $\mathcal{I}$ and $S$, and are then connected by NNLL renormalization group evolution that sums the jet-veto logarithms, which are encoded in ratios of these scales. The perturbative uncertainties can be assessed by considering two sources: i) an overall scale variation that simultaneously varies $\left\{\mu_{H}, \mu_{B}, \mu_{S}\right\}$ up and down by a factor of two which we denote by $\Delta_{H 0}$, and ii) individual variations of $\mu_{B}$ or $\mu_{S}$ that each hold the other two scales fixed [375], whose envelope we denote by the uncertainty $\Delta_{S B}$. Here $\Delta_{H 0}$ is dominated by the same sources of uncertainty as the total cross section $\sigma_{\text {total }}$, and hence should be considered $100 \%$ correlated with its uncertainty


Fig. 31: Relative uncertainties for the 0 -jet bin cross section from resummation at NNLL+NNLO for beam thrust $\mathcal{T}_{\mathrm{cm}}$ on the left and $p_{T}^{\text {jet }}$ on the right.
$\Delta_{\text {total }}$. The uncertainty $\Delta_{S B}$ is only present due to the jet-bin cut, and hence gives the $\Delta_{\text {cut }}$ uncertainty that is anti-correlated between neighboring jet bins.

If we simultaneously consider the cross sections $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ then the full correlation matrix in method C is

$$
C_{C}=\left(\begin{array}{cc}
\Delta_{S B}^{2} & -\Delta_{S B}^{2}  \tag{98}\\
-\Delta_{S B}^{2} & \Delta_{S B}^{2}
\end{array}\right)+\left(\begin{array}{cc}
\Delta_{H 0}^{2} & \Delta_{H 0} \Delta_{H \geq 1} \\
\Delta_{H 0} \Delta_{H \geq 1} & \Delta_{H \geq 1}^{2}
\end{array}\right),
$$

where $\Delta_{H \geq 1}=\Delta_{\text {total }}-\Delta_{H 0}$ encodes the $100 \%$ correlated component of the uncertainty for the ( $\geq 1$ )jet inclusive cross section. Computing the uncertainty in $\sigma_{\text {total }}$ gives back $\Delta_{\text {total }}$.

Eq. (98) can be compared to $C_{A}$ for method A in Eq. (95), which corresponds to taking $\Delta_{S B} \rightarrow 0$ and obtaining the analog of $\Delta_{H 0}$ by up/down scale variation without resummation ( $\mu_{H}=\mu_{B}=\mu_{S}$ ). It can also be compared to $C_{B}$ for method B in Eq. (97), which corresponds to taking $\Delta_{S B} \rightarrow \Delta_{\geq 1}$ and $\Delta_{H \geq 1} \rightarrow 0$, such that $\Delta_{H 0} \rightarrow \Delta_{\text {total }}$. The numerical dominance of $\Delta_{S B}^{2}$ over $\Delta_{H 0} \Delta_{H \geq 1}$ in the 0 -jet region is another way to justify the preference for using method B when only given a choice between methods A and B. For example, for $p_{T}^{\mathrm{cut}}=30 \mathrm{GeV}$ and $\left|\eta^{\text {jet }}\right| \leq 5.0$ we have $\Delta_{S B}^{2}=0.17$ and $\Delta_{H 0} \Delta_{H \geq 1}=0.02$.

In Fig. 31 we show the uncertainties $\Delta_{S B}$ (light green) and $\Delta_{H 0}$ (medium blue) as a function of the jet-veto variable, as well as the combined uncertainty adding these components in quadrature (dark orange). From the figure we see that the $\Delta_{H 0}$ dominates at large values where the veto is turned off and we approach the total cross section, and that the jet-cut uncertainty $\Delta_{S B}$ dominates for the small cut values that are typical of experimental analyses with Higgs jet bins. The same pattern is observed in the left panel which directly uses the NNLL+NNLO predictions for $\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$, and the right panel which shows the result from reweighting these predictions to $p_{T}^{\mathrm{cut}}$ as explained in Sec .12 .34 below.

### 12.34 Comparison of Uncertainty Methods

In Fig. 32 we compare the uncertainties for the 0 -jet bin cross section from methods A (medium green), B (light green), and C (dark orange). In the upper panels we use $\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$ as the jet-veto variable and full results for the NNLO and NNLL+NNLO cross sections, while in the lower panels we use $p_{T}^{\text {cut }}$ as the jet-veto variable with the full NNLO and the reweighted NNLL+NNLO results (as explained below). The upper panels use a cut on beam thrust, $\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$ while the lower panels use $p_{T}^{\mathrm{cut}}$. The right panels show the same results as those on the left, but are normalized to the highest-order result to better show the relative differences and uncertainties. The uncertainties in methods $\mathrm{A}, \mathrm{B}$, and C are computed from the upper left entry of the matrices $C_{A}, C_{B}$, and $C_{C}$, respectively.


Fig. 32: Comparison of uncertainties for methods A, B, C for the 0 -jet bin cross section for beam thrust $\mathcal{T}_{\text {cm }}$ (top) and $p_{T}^{\text {jet }}$ (bottom). Results are shown at NNLO with uncertainties from methods A and B and for the NNLL+NNLO resummed result using method C (reweighted for $p_{T}^{\mathrm{cut}}$ ). On the right all curves are normalized relative to the NNLL+NNLO central value.

From Fig. 32 we see that in method A (medium green bands) for small values of $p_{T}^{\text {cut }}$ the cancellations that take place in $\sigma_{0}\left(p^{\text {cut }}\right)$ cause the error bands to shrink and eventually almost vanish at $p_{T}^{\text {cut }} \simeq 25 \mathrm{GeV}$, where there is an almost exact cancellation between the two series in Eq. 88). This is avoided by using method B (light green bands). For large values of $p_{T}^{\text {cut }}$ method B reproduces the method A scale variation, since $\sigma_{\geq 1}\left(p^{\text {cut }}\right)$ becomes small. On the other hand, for small values of $p_{T}^{\text {cut }}$ the uncertainties estimated using method B are more realistic, because they explicitly estimate the uncertainties due to the presence of higher order large logarithmic corrections.

The features of this plot are quite generic. In particular, the same pattern of uncertainties is observed for the Tevatron, when using $\mu=m_{H}$ as our central scale (with $\mu=2 m_{H}$ and $\mu=m_{H} / 2$ for the range of scale variation), whether or not we only look at jets at central rapidities, or when considering the exclusive 1 -jet cross section. We also note that using independent variations for $\mu_{f}$ and $\mu_{r}$ does not change this picture, in particular the $\mu_{f}$ variation for fixed $\mu_{r}$ is quite small.

For method C with $\mathcal{T}_{\mathrm{cm}}$ we make use of resummed predictions for $H+0$ jets from gluon fusion at next-to-next-to-leading logarithmic order (NNLL+NNLO) from Ref. [375]. This includes the correct NNLO fixed-order corrections for $\sigma_{0}\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)$ for any cut. The resulting cross section $\sigma_{0}\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)$ has the jet veto implemented by a cut $\mathcal{T}_{\mathrm{cm}} \leq \mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$. This cross section contains a resummation of large logarithms at two orders beyond standard LL parton shower programs. A similar resummation for the case of $p_{T}^{\text {jet }}$ is not available. Instead, we use MC @ NLO and reweight it to the resummed predictions in $\mathcal{T}_{\mathrm{cm}}$, doing so for both the central curve as well as each of the six scale variation curves needed for the uncertainty


Fig. 33: In the left panel we show the same three curves as in the bottom-left panel of Fig. 32, but for the event fraction $f_{0}\left(p_{T}^{\mathrm{cut}}\right)$ treated as a derived quantity from the jet-bin cross sections. In the right panel we contrast the uncertainties obtained using Eqs. (92) and (93) together with method A, with the uncertainty obtained using method B.
determination in method $C{ }^{24}$ We then use the reweighted Monte Carlo sample to obtain cross section predictions for the standard jet veto, $\sigma_{0}\left(p_{T}^{\mathrm{cut}}\right)$. We will refer to this as the reweighted NNLL+NNLO result. Since the Monte Carlo here is only used to provide a transfer matrix between $\mathcal{T}_{\text {cm }}$ and $p_{T}^{\text {jet }}$, and both variables implement a jet veto, one expects that most of the improvements from the higherorder resummation are preserved by the reweighting. However, we caution that this is not equivalent to a complete NNLL+NNLO result for the $p_{T}^{\text {cut }}$ spectrum, since the reweighting may not fully capture effects associated with the choice of jet algorithm and other effects that enter at this order for $p_{T}^{\text {cut }}$. The dependence on the Monte Carlo transfer matrix also introduces an additional uncertainty, which should be studied and is not included in our numerical results. The transfer matrix is obtained at the parton level, without hadronization or underlying event, since we are reweighting a partonic NNLL+NNLO calculation.

From Fig. 32 one observes that the resummation of the large jet-veto logarithms (dark red central curve) lowers the cross section for both $\mathcal{T}_{\mathrm{cm}}^{\text {cut }}$ and $p_{T}^{\text {cut }}$. Comparing to NNLO for cut values $\gtrsim 25 \mathrm{GeV}$ the relative uncertainties in the resummed result of method C (dark orange bands) and the reduction in the resummed central value are similar for both jet-veto variables. Since one expects resummation to decrease the uncertainties, one can also see that the NNLO uncertainties from method B are more consistent with the higher order NNLL+NNLO resummed method C results than those in method A . We observe that the uncertainties in method C are reduced by about a factor of two compared to those in method B. Since the zero-jet bin plays a crucial role in the $H \rightarrow W W$ channel for Higgs searches, and these improvements will also be reflected in uncertainties for the one-jet bin, the improved theoretical precision obtained with method C has the potential to be quite important.

In Fig. 33 we show results for the 0 -jet event fraction $f_{0}$, with $p_{T}^{\text {cut }}$ as the jet-veto variable. In the left panel we compare the uncertainties in $f_{0}\left(p_{T}^{\text {cut }}\right)$ that result from propagating the uncertainties from the jet-bin cross sections obtained from methods A (medium green), B (light green), and C (dark orange). The conclusions are analogous to the corresponding cross-section results in the bottom-left panel of Fig. 32, namely that method B provides a better estimate for the perturbative fixed-order uncertainties than method A, and that the higher-order logarithmic summation present in method C leads to a slightly smaller central value together with the decrease to the uncertainty one expects from incorporating the resummation. In the right panel of Fig. 33 we show the results of the different perturbative schemes for $f_{0}$ defined in Eq. 92) (middle dark green band) and Eq. 93) (lower narrow blue band and upper wide

[^134]|  | method A | method B | method C |
| :---: | :---: | :---: | :---: |
| $\delta \sigma_{0}\left(p_{T}^{\text {cut }}\right)$ | $3 \%$ | $19 \%$ | $9 \%$ |
| $\delta \sigma_{\geq 1}\left(p_{T}^{\text {cut }}\right)$ | $19 \%$ | $19 \%$ | $14 \%$ |
| $\rho\left(\sigma_{\text {total }}, \sigma_{0}\right)$ | 1 | 0.78 | 0.15 |
| $\rho\left(\sigma_{\text {total }}, \sigma_{\geq 1}\right)$ | 1 | 0 | 0.65 |
| $\rho\left(\sigma_{0}, \sigma_{\geq 1}\right)$ | 1 | -0.63 | -0.65 |
| $\delta f_{0}\left(p_{T}^{\text {cut }}\right)$ | $6 \%$ | $13 \%$ | $9 \%$ |
| $\delta f_{\geq 1}\left(p_{T}^{\text {cut }}\right)$ | $10 \%$ | $21 \%$ | $11 \%$ |
| $\rho\left(\sigma_{\text {total }}, f_{0}\right)$ | -1 | 0.43 | -0.38 |
| $\rho\left(\sigma_{\text {total }}, f_{\geq 1}\right)$ | 1 | -0.43 | 0.38 |

Table 9: Example of relative uncertainties $\delta$ and correlations $\rho$ obtained for the LHC at 7 TeV for $p_{T}^{\text {cut }}=$ 30 GeV and $\left|\eta^{\text {jet }}\right| \leq 5.0$.
yellow band) each at NNLO and in each case obtaining the uncertainties using method A (direct scale variation) [376](Sec. 5.3). For comparison, the middle light green band shows the uncertainties obtained from method B. The different method A schemes have a wide spread, which demonstrates the large size of the higher-order perturbative corrections in the total and inclusive 1-jet cross sections. The central values of the alternative methods $A_{2}$ and $A_{3}$ are not covered by the method $A_{1}$ uncertainty band, but all three central curves are covered by the larger uncertainty band from method B (except at small $p_{T}^{\text {cut }}$ where scheme 3 starts to diverge earlier than the other schemes). This can be taken as a confirmation that method A tends to underestimate the perturbative uncertainties in the fixed-order results [376](Sec. 5.3), while method B produces more realistic fixed-order uncertainties.

To appreciate the effects of the different methods on the correlation matrix we consider as an example the results for $p_{T}^{\text {cut }}=30 \mathrm{GeV}$ and $\left|\eta^{\text {jet }}\right| \leq 5.0$. The inclusive cross sections are $\sigma_{\text {total }}=(8.76 \pm$ $0.80) \mathrm{pb}$ at NNLO, and $\sigma_{\geq 1}=(3.31 \pm 0.64) \mathrm{pb}$ at NLO. The relative uncertainties and correlations at these cuts for the three methods are shown in Table 9 . The numbers for the cross sections are also translated into the equivalent results for the event fractions, $f_{0}\left(p_{T}^{\text {cut }}\right)=\sigma_{0}\left(p_{T}^{\text {cut }}\right) / \sigma_{\text {total }}$ and $f \geq 1\left(p_{T}^{\text {cut }}\right)=$ $\sigma_{\geq 1}\left(p_{T}^{\text {cut }}\right) / \sigma_{\text {total }}$. Note that method A should not be used due to the lack of a contribution corresponding to $\Delta_{\text {cut }}$ in this method, and the resulting underestimated $\delta \sigma_{0}$. In methods B and C we see, as expected, that $\sigma_{0}$ and $\sigma_{\geq 1}$ have a substantial anti-correlation due to the jet-bin boundary they share.

### 12.4 Conclusion

To summarize, we have discussed the implications of separating LHC cross sections into jet bins, using Higgs production from gluon fusion as a concrete example. The jet binning induces logarithmic dependences on the jet-bin boundary which is important to properly take into account when making predictions and estimating perturbative uncertainties. When using fixed-order predictions only, the additional logarithms at higher orders in perturbation theory caused by the jet binning can be taken into account in the perturbative uncertainty estimate using method B. By resumming the jet-binning logarithms one can obtain improved predictions with reduced (and more sophisticated) uncertainties using method C.

Here we have focused our discussion on $\sigma_{0}$ and $\sigma_{\geq 1}$ and how to take into account the resulting jet-bin boundary. To further separate $\sigma_{\geq 1}$ into a one-jet bin $\sigma_{1}$ and a $\sigma_{\geq 2}$ one can use method B for this boundary by treating $\Delta_{\geq 2}$ as uncorrelated with the total uncertainty for $\sigma_{\geq 1}$ from either methods B or C. Examples of utilizing method B for this jet bin boundary can be found in Ref. [26]. Once it becomes available one can also use a resummed prediction with uncertainties for this boundary with method C .

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## 13. A NLO BENCHMARK COMPARISON FOR INCLUSIVE JET PRODUCTION AT HADRON COLLIDERS ${ }^{25}$


#### Abstract

We present a benchmark comparison of two next-to-leading order (NLO) calculations for inclusive jet and jet pair production at hadron colliders. A new version of the NLO code EKS is adapted for computation of differential cross sections and compared to an independent calculation based on the FastNLO code. A percent-level agreement between the two codes is observed for specified settings of computations at typical transverse momenta and rapidities of Tevatron and LHC measurements. We identify theoretical prerequisites for achieving such level of agreement and comment on the stability of NLO calculations with respect to the factorization scale choice.


### 13.1 INTRODUCTION

Inclusive jet production at hadron colliders provides an excellent opportunity to test perturbative QCD (PQCD) and look for possible new physics beyond the Standard Model (SM) over a wide range of energy scales. Single inclusive jet production in the Tevatron Run-2 has been recently used to determine the QCD coupling constant [377] and constrain parton distribution functions (PDF) in the proton in global QCD analyses by several groups [255, 378, 262, 311]. Jet production data provide constraints on the gluon PDF at large $x$ values, possibly in a combination with small- $x$ quark PDFs, as discussed in Section 7. Invariant mass distributions of dijets [379], angular distributions [380, 381], and other jet observables at the LHC [382, 293, 292] provide a unprecedented opportunity to extend searches for quark compositeness and new particle resonances toward the highest energies attainable.

In this contribution, we examine agreement between the computer programs that are available for NLO calculations of jet production cross sections. NLO QCD predictions for jet production work remarkably well in a wide kinematical range and across many orders of magnitude of the cross sections. Nonetheless, the latest PDF analysis evaluates many scattering processes up to NNLO in perturbative QCD. Jet production observables are pivotal for constraining the large- $x$ gluon PDF, but remain known to NLO only. We identify and document main factors affecting NLO jet cross sections at a few-percent level of accuracy and compare the numerical results for typical collider kinematics. Differences between the programs used, and choices for the theoretical inputs made, may be responsible for some differences observed between CT10 and other PDFs, as explained below. Such NLO benchmark comparison will be useful for quantifying or reducing the uncertainties on the resulting PDFs and for the future implementation of NNLO and higher-order resummed contributions to the jet cross sections.

From the experimental point of view, jet production has an advantage of very high statistics and a drawback of sizeable systematical errors associated with complexities of jet reconstruction. NLO theoretical uncertainties due to the QCD scale dependence and the fixed-order model for the jet algorithm are comparable to the experimental errors. Control of numerical accuracy involves, in particular, careful tuning of Monte-Carlo integration to handle steeply falling jet cross sections.

An early numerical code (EKS) for the NLO calculation of single-inclusive jet and dijet distributions was developed by S. D. Ellis, Z. Kunszt and D. E. Soper in 1990's [383] based on the subtraction method. Two other widely used numerical programs are NLOJET++ [384, 385] and FastNLO [290, 291].

[^135]The latter provides a fast interface to obtain NLO predictions in kinematical bins of already published experimental jet cross sections by interpolating table files produced by NLOJET++. Besides these fixedorder calculations, POWHEG combines the NLO jet production cross sections with leading-logarithm QCD showering effects [386]. Some phenomenological studies also include partial NNLO contributions to jet cross sections obtained by threshold resummation [387].

The agreement between the above NLO numerical programs is not automatically met, which motivates the present benchmark comparison. The past CTEQ PDF analyses computed NLO jet cross sections using NLO K-factor tables produced by the EKS code, while other PDF analysis groups use FastNLO. Since the CT10 NLO gluon PDF behaves somewhat differently at large $x$ than the gluon PDF from MSTW'08 or other groups [262], one must compare the EKS and FastNLO computations for the same input values to confirm that these programs do not cause the observed disagreement.

Here we show that the results for the Tevatron $(\sqrt{s}=1.96 \mathrm{TeV})$ and LHC $(\sqrt{s}=7 \mathrm{TeV})$ from EKS and FastNLO agree well when the computation parameters are chosen as described in the next section. These settings must be consciously controlled in order to reach acceptable agreement. As a result of this work, the EKS code has been revised to improve its stability and efficiency and to implement output into new differential cross sections [388].

### 13.2 Theoretical setup and inputs

Several theoretical inputs must be matched exactly between the EKS and FastNLO programs in order to reach the level of agreement shown in the figures below.

- Jet algorithm. When calculating the distribution of jet observables, we need to use the same jet algorithms as the ones in the experimental measurements. In this comparison, we utilized the cone-based Midpoint algorithm [389] for the Tevatron observables and cluster-based anti- $k_{T}$ algorithm [341] for the LHC. The only difference between the Midpoint algorithm and modified Snowmass algorithm [389] used in the original EKS program is that the Midpoint algorithm always starts with the middle point between the two partons' directions as a seed for a new protojet, no matter how large their separation is. In the NLO theoretical calculations for single-jet or dijet production that include at most three final-state partons, the cluster-based $k_{T}$ [390], anti- $k_{T}$, and Cambridge-Aachen (CA) [391] algorithms are equivalent.
- The recombination scheme is a procedure for merging two nearby partons into one jet. For example, the energy scheme (4D, based on adding the 4-momentum) or $E_{T}$ scheme (based on adding the scalar $E_{T}$, then averaging over the partons' directions using $E_{T}$ as the weights) can be employed to find the momentum of the merged jet [392]. Our comparison uses the energy scheme for both the Tevatron and LHC measurements, as it is often used by the recent experiments. Different choices of the recombination scheme can cause differences of up to ten percent in the NLO distributions, as will be shown later. Note that, with the energy scheme, the jet could be massive, which means that the jet's pseudorapidity will not be equal to its rapidity.
- The jet trigger imposes acceptance conditions on each jet's $p_{T}$ or rapidity when deciding if this jet's contribution is included into the jet observable. In NLO calculations of single-inclusive jet distributions, the jet trigger conditions have no influence. In dijet production, they may change the cross sections by small amounts by affecting the selection of two leading jets in some cases. In our dijet calculations we choose $p_{T}>40 \mathrm{GeV},|y|<3$ for each jet at the Tevatron and $p_{T}>30 \mathrm{GeV}$, $|y|<3$ at the LHC.
- Renormalization and factorization scales. The scale choice is only related to theory and has no correspondence in experiment. It is conventional to choose the renormalization and factorization scales to be of order of the typical transverse momentum $p_{T}$ of the jet(s): $\mu_{R} \sim \mu_{F} \sim p_{T}$. In contributions with two resolved jets, $p_{T}$ naturally corresponds to the transverse momentum of either of the final-state jets (which are equal by momentum conservation). More ambiguity
is present in contributions with three resolved jets, when $p_{T}$ can correspond to the transverse momentum of either of the jets in each event or to a combination of three transverse momenta. A meaningful comparison must use equivalent definitions of " $j$ et $p_{T}$ " in the renormalization and factorization scales of both NLO calculations.
When FastNLO interpolates tables of NLOJET++ cross sections for single inclusive-jet production, it sets $\mu_{R}$ and $\mu_{F}$ proportional to the $p_{T}$ value at a fixed point in each $p_{T}$ bin of the experimental data. Given the high precision of the latest PDF analyses, the FastNLO scale convention produces a numerically different result than the scale proportional to the $p_{T}$ of the leading jet or the average $p_{T}$ of two leading jets in each event. It depends on the binning of the experimental data and is numerically close to the average $p_{T}$ in each bin for small enough bins.
In the EKS calculations for single-jet production, we set the scale proportional to $p_{T}$ of each individual jet in any $p_{T}$ bin, which means that we repeat the evaluation of the matrix elements with three resolved jets (contributing to three $p_{T}$ bins) by successively setting $\mu_{R, F}$ to be proportional to the $p_{T}$ of each jet in the event. Such matrix elements are thus evaluated three times. This event-level scale setting of EKS turns out to be numerically close to the bin-level scale setting of FastNLO if the bin sizes are small. However, a few-percent differences are still observed at the largest rapidities and $p_{T}$. For dijet production, FastNLO and EKS choose the $\mu_{R}$ and $\mu_{F}$ scales that are proportional to the average $\left|p_{T}\right|=\left(\left|p_{T 1}\right|+\left|p_{T 2}\right|\right) / 2$ of the two leading jets.
- Monte-Carlo integration. Precision calculations for jet production are numerically challenging because of the rapid falloff of the cross sections with the jet's $p_{T}$ and rapidity, and also because of large numerical cancellations occurring between some $2 \rightarrow 2$ and $2 \rightarrow 3$ contributions. Both EKS and NLOJET ++ evaluate differential cross sections by Monte-Carlo integration, which requires to generate of order $10^{9}$ of sample points to achieve percent-level accuracy for the whole kinematical region. The upgraded EKS code performs the Monte-Carlo integration using the VEGAS method from the CUBA2.1 library [393]. The EKS output is produced in the form of two-dimensional cross sections ( $\left.d^{2} \sigma /\left(d p_{T} d y\right), d^{2} \sigma /\left(d M_{j j} d y\right), \ldots\right)$ and stored in finely binned two-dimensional histograms. Such output is "almost fully differential" in the sense that the finely grained histograms can be rebinned into any set of coarse bins of the given experiment at the stage of the user's final analysis. This format is different from the FastNLO format, which provides the cross sections in coarse bins taken from pre-existing experimental publications.
The fine binning in EKS is introduced at the stage of Monte-Carlo integration in order to improve convergence and to better handle the NLO cancellations. The Monte Carlo sampling pattern is tuned automatically to ensure that all fine bins are filled with comparable numbers of sample points, regardless of the momentum and scattering angle values associated with each bin. Then we get uniform relative errors on the cross sections in all bins without consuming too much CPU time, and despite the dramatic variation of cross sections across the bins. Finally, EKS includes a module to allow for flexible choices of scales $\mu_{R}$ and $\mu_{F}$, and another module for calculating differential cross sections of user-provided jet observables.


### 13.3 RESULTS

Figs. 3439 compare our representative numerical results with the ones provided by FastNLO for $p_{T}$ distributions of single jets, invariant mass distributions of dijets, and (in the case of D0 Run-2) angular distributions ( $\chi$ ) of dijets. Kinematical bins of the Tevatron $(\sqrt{s}=1.96 \mathrm{TeV}$ ) [287, 285, 289, 394] and LHC $(\sqrt{s}=7 \mathrm{TeV})$ [293, 292] measurements, and CTEQ6.6 PDFs [256] were used. The cone sizes $R$ of the jets are indicated in the figures.

Left panels in the figures show ratios of EKS to FastNLO cross sections, $\sigma_{\text {EKS }} / \sigma_{\text {FastNLO }}$, at the LO (red points) and $\mathrm{NLO}=\mathrm{LO}+\mathrm{NLO}$ correction (blue points), in kinematical bins provided by the experiments. The horizontal axis indicates the ID of each bin, which are arranged in the order of increasing jet rapidity $y$ and then jet's $p_{T}$ for inclusive jet production, $y$ and then $M_{j j}$ for dijet production, and $M_{j j}$
then $\chi$ for dijet angular dependence. Vertical lines indicate the boundaries of each rapidity interval for single-jet and dijet distributions, and of each dimass interval for the $\chi$ distribution. For example, Fig. 34 shows $\sigma_{\text {EKS }} / \sigma_{\text {FastNLO }}$ in 6 bins of jet rapidity, with bins $1 . . .23$ corresponding to the first rapidity bin ( $|y|<0.4$ ), bins $24 \ldots 45$ corresponding to the second rapidity bin $(0.4<|y|<0.8$ ), and so on.

The left panel includes, from top to bottom, three plots obtained with the renormalization and factorization scales equal to $1 / 2,1$, and 2 times the center scale. We can see a good overall agreement between EKS and FastNLO both at LO and NLO. The only significant discrepancies are found in the highest $p_{T}$ bins for both the Tevatron and LHC single inclusive jet production, which may be due to the difference in the scale choices used in EKS and FastNLO. [These differences reduce when going to NLO]. In the EKS single-jet calculation, we use the actual $p_{T}$ of the partonic jet filled into the bin as the scale input. FastNLO sets the scale according to a fixed $p_{T}$ value in each experimental bin, which tends to be different from the EKS scale in the highest $p_{T}$ bins, which have large widths. The same reason causes a small normalization shift in the other $p_{T}$ bins.

For dijet production, we only observe random fluctuations at highest $M_{j j}$ that are mainly due to numerical integration errors.

In the right panels of Figs. 34 39, we present plots of the NLO K factor from EKS for each distribution, defined as the ratio of the NLO differential cross section to the LO one. The value of the K factor and its stability with respect to the scale choice may provide an indication of the magnitude of yet higher-order corrections.

To minimize the potential effect of higher-order terms, one might opt to choose the renormalization and factorization scales that bring the K factor close to unity in most of the kinematical region. An alternative approach for setting the scale is based on the minimal sensitivity method, which suggests to choose the $\mu_{R}$ and $\mu_{F}$ values (taken to be equal and designated as $\mu$ in the following) at the point where the scale dependence of the NLO cross section is the smallest.

In (di)jet production at central rapidities at the Tevatron, both requirements ( $K \approx 1$ and $d \sigma_{N L O}(\mu) / d \mu \approx 0$ ) could be satisfied by choosing $\mu \approx 0.5 p_{T}$; see, e.g., the appendix in Ref. [395]. For this reason, the scale $p_{T} / 2$ was used in the CT10 study. However, the point of the minimal sensitivity shifts to higher values (close to $p_{T}$ or even higher) at forward rapidities at the Tevatron or at all rapidities at the LHC. For such higher scales, however, it is hard to satisfy the requirement that $K$ remains close to unity at the same time.

This point is illustrated by our plots of the $K$ factors. At the central rapidities and $\mu_{R}=\mu_{F}=$ $0.5 p_{T}$ at the Tevatron (the lowest 3 rapidity bins in Figs. 34.37), $K \approx 1$ and is relatively independent of $p_{T}$, as seen in the top subpanels. However, with this scale choice the K factor deviates significantly from unity and has strong kinematic dependence if the rapidity and $p_{T}$ are large. If one chooses the scale that is equal to $p_{T}$ or even $2 p_{T}$ (the middle and bottom figures), in accord with the minimal sensitivity method for the forward bins, the kinematical dependence of the K factor reduces, but its value increases to 1.3-1.6 in most of the bins.

For CMS kinematics (Figs. 38|39), the $K$ factor has significant kinematical dependence for all central scale choices, however, the choice $\mu_{R}=\mu_{F}=p_{T}$ (the middle subpanels) results in a comparatively flatter $K$ factor that is also closer to unity. We can see that it is hard to find a fixed scale (or a scale of the type $p_{T} \times($ a function of $y)$ [383]) that would simultaneously reduce the magnitude of the NLO correction and stabilize its scale dependence and kinematical dependence. The scale $0.5 p_{T}$ may be slightly more optimal at the Tevatron, and the scale $p_{T}$ may be slightly better at the LHC. In the absence of a clearly superior scale choice, it may be necessary to vary the scale of jet cross sections in the global fit in order to estimate its effect on the PDF errors.

In Figs. 40 and 41, we plot the ratios of the NLO distributions calculated using different recombination schemes, where $\sigma_{4 D}$ is obtained with the energy scheme, and $\sigma_{E_{T}}$ is with the $E_{T}$ scheme. For single inclusive jet production at both the Tevatron and LHC, $\sigma_{E_{T}}$ is larger then $\sigma_{4 D}$. An opposite trend
is observed in dijet production. Differences of the predictions based on the two schemes are larger with the Midpoint algorithm (used at the Tevatron) than with the anti- $k_{T}$ algorithm (used at the LHC). In an NLO calculation, the Midpoint algorithm allows a larger maximal angular separation $(2 R)$ between the two partons forming a jet, compared to the anti- $k_{T}$ algorithm that only allows the angular separation up to $R$. This produces the shown kinematical differences between the two schemes.

## CONCLUSIONS

Jet production plays an important role at hadron colliders and is a main background process in the bulk of new physics searches. A benchmark comparison of NLO QCD predictions for jet production from different numerical codes can be useful for both the ongoing phenomenological studies and upcoming higher-order calculations. In this work we modify the original EKS program and compare the singlejet and dijet cross sections that it produces with the ones from the FastNLO program. We find a good agreement between two programs, apart from differences of up to $5-10 \%$ occuring at the highest jet $p_{T}$ 's and rapidities. We document the exact combination of theoretical settings in EKS that are needed to reproduce the FastNLO results. Based on the EKS calculation, we attempted to identify the choice of the renormalization and factorization scales that could simultaneously reduce the magnitude of NLO $K$ factors and/or scale dependence of the NLO cross section. Since we could not easily find such a scale combination, we propose to vary the factorization and renormalization scales in future (N)NLO PDF fits to better estimate theoretical uncertainties in the resulting PDFs. There is a plan to publish the updated EKS program in the near future [388].

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Fig. 34: Comparison of $p_{T}$ distributions for single inclusive jet production from EKS and FastNLO for D0 Tevatron Run II measurement.[287]


Fig. 35: Comparison of $p_{T}$ distributions for single inclusive jet production from EKS and FastNLO for CDF Tevatron Run II measurement. [285]


Fig. 36: Comparison of invariant mass distributions for dijet production from EKS and FastNLO for D0 Tevatron Run II measurement.[289]


Fig. 37: Comparison of angular $(\chi)$ distributions for dijet production from EKS and FastNLO for D0 Tevatron Run II measurement.[394]


Fig. 38: Comparison of $p_{T}$ distributions for single inclusive jet production from EKS and FastNLO for CMS LHC ( 7 TeV ) measurement. [292]


Fig. 39: Comparison of invariant mass distributions for dijet production from EKS and FastNLO for CMS LHC ( 7 TeV ) measurement. [293]


Fig. 40: Comparison of $p_{T}$ distributions for single inclusive jet production using different recombination schemes.


Fig. 41: Comparison of invariant mass distributions for the dijet production using different recombination schemes.

## 14. PHENOMENOLOGICAL STUDIES WITH AMC@ NLO ${ }^{26}$


#### Abstract

We present four phenomenological studies of hadron collider processes performed within the aMC @ NLO framework


### 14.1 Introduction

aMC@NLO (http://amcatnlo.cern.ch) is a fully automated approach to complete event generation and subsequent parton shower at the NLO accuracy in QCD, which allows accurate and flexible simulations for both signals and backgrounds at hadron colliders. All calculational aspects in aMC @ NLO are automated. One-loop contributions are evaluated with MadLoop [8, 396], that uses the OPP integrand reduction method [121] as implemented in CutTools [135]. The other matrix-element contributions to the cross sections, their phase-space subtractions according to the FKS formalism [397], their combinations with the one-loop results, and their integration are performed by MadFKS [398] ${ }^{27}$. The matching of the NLO results with HERWIG [399] or PYTHIA [400] parton showers is performed with the MC@NLO method [401], and it is also completely automatic. Finally, aMC @ NLO can compute scale and PDF uncertainties at no extra CPU-time cost with the help of the process-independent reweighting technique described in [402].

For all technical details we refer to the original publications. We report here on the physics results obtained with aMC @ NLO for observables of interest at hadron colliders [15, 403, 402, 404]. We stress that they are simulated at the hadron level, namely including parton shower and hadronization effects. In Sects. 14.2, 14.3, and 14.4 we present results for the production of $t t H, V b b$, and four-lepton final states at the LHC, respectively. Section 14.5 reports on a study of the $W j j$ process at Tevatron. Finally, in sect. 14.6 we draw our conclusions. The list of the processes considered here should convince the reader that one can perform realistic analyses of experimental data, for signals and backgrounds, entirely within the aMC@NLO framework.

### 14.2 The $t t H$ process at the LHC

The production process of a $H$ boson in association with a top pair [15] is a classic mechanism for Higgs production at the LHC [24, 405], where the large $t t H$ Yukawa coupling and the presence of top quarks can be exploited to extract the signal from its QCD multi-jet background. As an example of the use of aMC @ NLO for this process we present, in Fig. 42, the Higgs transverse momentum distribution and the transverse momentum of the $t t H$ or $t t A$ system at the $\sqrt{s}=7 \mathrm{TeV}$ LHC for a Standard Model (scalar) Higgs with $M_{H}=120 \mathrm{GeV}$ and for a pseudoscalar one with $M_{A}=120 / 40 \mathrm{GeV}$. The total NLO cross sections in the three cases are $\sigma_{\mathrm{NLO}}\left(M_{H}=120\right)=103.4 \mathrm{fb}, \sigma_{\mathrm{NLO}}\left(M_{A}=120\right)=31.9 \mathrm{fb}$, and $\sigma_{\mathrm{NLO}}\left(M_{A}=40\right)=77.3 \mathrm{fb}$, respectively. At moderate values of the Higgs transverse momentum, the scalar and pseudoscalar cases are clearly distinguishable, while at larger values the three distributions tend to coincide. Parton shower effects give in general small corrections with respect to the a pure NLO calculation, except for variables involving all produced particles, such as the transverse momentum of the $t t H$ or $t t A$ system shown in the right panel of Fig. 42.

### 14.3 The $V b b$ process at the LHC

With $V b b$ we understand $\ell \nu b b$ and $\ell^{+} \ell^{-} b b$ final states [403], which are the main backgrounds to searches for SM Higgs production in association with vector bosons $(W H / Z H)$, with the subsequent Higgs decay into a $b b$ pair. The aMC @ NLO framework allows a realistic study including

- NLO corrections;

[^136]

Fig. 42: Higgs transverse momentum distributions (left) and transverse momentum of the $t t H$ or $t t A$ system (right) in $t t H / t t A$ events at the LHC ( $\sqrt{s}=7 \mathrm{TeV}$ ), with aMC @ NLO in the three cases: Scalar (blue) and pseudoscalar (magenta) Higgs with $m_{H / A}=120 \mathrm{GeV}$ and pseudoscalar (green) with $m_{A}=$ 40 GeV . In the lower panels of the left part, the ratios of aMC @ NLO over LO (dashed), NLO (solid), and aMC@LO (crosses) are shown. Solid histograms in the right panel are relevant to aMC@NLO, dashed ones to a pure NLO calculation.

- bottom quark mass effects;
- spin-correlation and off-shell effects;
- showering and hadronization.

As an example we show, in Fig. 43, the invariant mass of the pair of the two leading b-jets, compared with the signal distributions for a standard Higgs with $m_{H}=120 \mathrm{GeV}$. Fig. 43 is interesting because both signal and background are studied at the NLO accuracy. It should be noted that, since completely hadronized events are simulated, sophisticated studies of the jet sub-structure are possible within the aMC@NLO framework, as presented in Fig. 44 , where the fractions of events containing zero $b$-jets, exactly one $b$-jet, and exactly two $b$-jets are plotted. The $b$-jet fractions are fairly similar for $W b b$ and $Z b b$ production, and the effects of the NLO corrections are consistent with the fully-inclusive $K$ factors. On the other hand, the $b b$-jet contribution to the $b$-jet rate is seen to be more than three times larger for $\ell^{ \pm} \nu b b$ than for $\ell^{+} \ell^{-} b b$ final states. This fact is related to the different mechanisms for the production of a $b b$ pair in the two processes. At variance with the case of $\ell^{ \pm} \nu b b$ production, in a $\ell^{+} \ell^{-} b b$ final state the two $b$ 's may come from the separate branchings of two initial-state gluons, and thus the probability of them ending in the same jet is much smaller than in the case of a $g \rightarrow b b$ final-state branching, which gives the only possible contribution to a $\ell^{ \pm} \nu b b$ final state.

### 14.4 Four-lepton production at the LHC

Vector boson pair production is interesting in at least two respects. Firstly, it is an irreducible background to Higgs signals, in particular through the $W^{+} W$ and $Z Z$ channels which are relevant to searches for a standard model Higgs of mass larger than about 140 GeV . Secondly, di-boson cross sections are quite sensitive to violations of the gauge structure of the Standard Model, and hence are good probes of scenarios where new physics is heavy and not directly accessible at the LHC, yet the couplings in the vector boson sector are affected. We consider here the neutral process [402]

$$
p p \rightarrow\left(Z / \gamma^{*}\right)\left(Z / \gamma^{*}\right) \rightarrow \ell^{+} \ell^{-} \ell^{(\prime)+} \ell^{(\prime)-},
$$



Fig. 43: Invariant mass of the pair of the two leading $b$-jets. $W H(\rightarrow \ell \nu b b), Z H\left(\rightarrow \ell^{+} \ell^{-} b b\right), \ell \nu b b$, and $\ell^{+} \ell^{-} b b$ results are shown, with the former two rescaled by a factor of ten.

| Process | Cross section (fb) |  |  |
| :---: | :---: | :---: | :---: |
|  | $q \bar{q} / q g$ channels |  |  |
|  | $\mathcal{O}\left(\alpha_{s}^{0}\right)$ | $\mathcal{O}\left(\alpha_{s}^{0}\right)+\mathcal{O}\left(\alpha_{s}\right)$ | $g g$ channel |
| $p p \rightarrow e^{+} e^{-} \mu^{+} \mu^{-}$ | 9.19 | $12.90_{-0.23(1.8 \%)-0.22(1.7 \%)}^{+0.27(2.1 \%)+0.26(2.0 \%)}$ | $0.566_{-0.118(20.8 \%)-0.014(2.5 \%)}^{+0.162(28.5 \%)+0.012(2.1 \%)}$ |
| $p p \rightarrow e^{+} e^{-} e^{+} e^{-}$ | 4.58 | $6.43_{-0.13(2.0 \%)-0.10(1.6 \%)}^{+0.13(2.1 \%)+0.1(1.7)}$ |  |

Table 10: Total cross sections for $e^{+} e^{-} \mu^{+} \mu^{-}$and $e^{+} e^{-} e^{+} e^{-}$production at the $\mathrm{LHC}(\sqrt{S}=7 \mathrm{TeV})$ within the cuts $M\left(\ell^{ \pm} \ell^{(1) \mp}\right) \geq 30 \mathrm{GeV}$. The first and second errors affecting the results are the scale and PDF uncertainties (also given as fractions of the central values).
which, although smaller than the $W^{+} W^{-}$channel, may provide a cleaner signal due to the possibility of fully reconstructing the decay products of the two vector bosons. aMC @ NLO predictions for the cross sections are given in Tab. 10, which also includes aMC @ NLO estimates for scale and PDF uncertainties. The four-lepton invariant mass and the transverse momentum distribution are presented in Fig. 45, where comparisons between the results obtained with aMC @ NLO matched to HERWIG and to PYTHIA are also given. We stress that these results include the contributions due to $g g$-initiated processes, which have also been computed automatically. These are formally of NNLO, but may play a non-negligible phenomenological role owing to their parton-luminosity dominance at a large-energy collider such as the LHC.

### 14.5 Wjj at Tevatron

In [406] CDF reported an excess of events in two-jet production in association with a $W$ boson, in the form of a broad peak centered at $M_{j j}=144 \mathrm{GeV}$ in the dijet invariant mass ${ }^{28}$. Motivated by this fact, we present in Fig. 46]the aMC @ NLO prediction [404] for the dijet invariant mass in $W j j$ events, using the same cuts as CDF and D0 in the signal region, also comparing with a pure NLO computation and with the Alpgen [408] findings (one-, two-, and three-parton multiplicities have been consistently matched to

[^137]

Fig. 44: Fractions of events (in percent) that contain: zero $b$-jets, exactly one $b$-jet, and exactly two $b$-jets. The rightmost bin displays the fraction of $b$-jets which are $b b$-jets. The two insets show the ratio of the aMC @ NLO results over the corresponding NLO (solid), aMC @ LO (dashed), and LO (symbols) ones, separately for $W b b$ (upper inset) and $Z b b$ (lower inset) production.
obtain the latter). Perturbative, parton-level results agree well with those obtained after shower, and PDF and scale uncertainties (also reported in Fig. 46) are well under control. In summary, we do not observe any significant effects in the shape of distributions due to NLO corrections, which therefore cannot be responsible for the excess of events observed by the CDF collaboration.

### 14.6 Conclusions

The results we have presented in this contribution are based on the strategic assumption that, for the word automation to have its proper meaning, the only operation required from a user is that of typing-in the process to be computed, and other analysis-related information (such as final-state cuts). In particular, the codes that achieve the automation may only differentiate between processes depending on their general characteristics, but must never work on a case-by-case basis. The aMC@NLO framework is based on such an assumption, providing a very powerful tool to compare, at the NLO accuracy including showering and hadronization, theory and experiment in high energy collisions. As an example of the flexibility of aMC@NLO we have presented results for the processes $p p \rightarrow t t H, p p \rightarrow V b b, p p \rightarrow$ $\ell^{+} \ell^{-} \ell^{(1)+} \ell^{(1)-}$ at the LHC, and a study of $p \bar{p} \rightarrow W j j$ at Tevatron.

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## 15. PROBING CORRECTIONS TO DIJET PRODUCTION AT THE LHC ${ }^{29}$

## Abstract

We compare and discuss a few kinematic distributions for dijet production at the LHC, computed with a fixed next-to-leading order code, with the

[^138]

Fig. 45: Four-lepton invariant mass and the transverse momentum distributions for aMC@NLO $+g g$ HERWIG (solid black) and PYTHIA (dashed blue) results. The rescaled $g g$ contributions with HERWIG (open black boxes) and PYTHIA (open blue circles) are shown separately. Middle insets: scale (dashed red) and PDF (solid black) fractional uncertainties. Lower insets: aMC@NLO/(aMC@NLO+gg) with HERWIG (solid black) and PYTHIA (dashed blue).

POWHEG BOX and with HEJ. Previous experimental studies have dealt with kinematic distributions where the predictions of the three approaches were very similar. In this proceeding, we investigate kinematic distributions where the resummed effects in POWHEG and HEJ are clearly shown and enhanced with respect to the fixed NLO result, since different QCD-radiation regimes are probed.

### 15.1 Introduction

Dijet production is one of the cornerstone processes at the LHC. The cross section for jet production is very large, making it an important testing ground for our understanding of QCD at high-energy scales. In addition, jet production is an important background for many searches for new physics. It is therefore essential to probe and test our theoretical predictions. Dijet-production studies can bring insights in jet production in association with other particles too: for example, Higgs boson production plus two jets in gluon fusion, a key process for assessing the CP properties of the Higgs boson, can benefit from these studies.

There have been a number of very interesting experimental studies in dijet production by both the ATLAS [410, 411, 294] and CMS [412, 413, 414, 415] Collaborations. It is already clear that higher order QCD contributions beyond a fixed order, low multiplicity calculation can be important because the large available phase space for jet emission at the LHC compensates for the suppression of extra powers of the strong coupling constant.

In this contribution, we compare two theoretical approaches to dijet production that include higher order effects: POWHEG [416, 417, 386, 13] and HEJ [418, 419, 64]. The POWHEG method successfully merges a fixed next-to-leading order (NLO) calculation with a parton shower program, that resums leading logarithmic contributions from collinear emissions. In this study, the POWHEG results obtained with the POWHEG BOX [13] are interfaced with the transverse-momentum-ordered shower


Fig. 46: Invariant mass of the pair of the two hardest jets, with CDF/D0 cuts of [406] (left) and of [409] (right).
provided by PYTHIA 6.4.21 [400]. In contrast, the starting point for HEJ is an all-order approximation to the hard scattering matrix element in the regime of wide-angle QCD emissions. HEJ is accurate at leading logarithmic precision in the invariant mass of any two jets. This is then supplemented with the missing contributions (through a merging and reweighting-procedure) necessary to also ensure tree-level accuracy for final states with up to four jets. The tree-level matrix elements are taken from Standalone Madgraph [163].

The POWHEG and HEJ approaches are clearly very different in their description of QCD radiation. Nevertheless, for several kinematic distributions (see for example ref. [410]) the predictions from POWHEG and HEJ are very similar. In this study, we investigate various observables which can expose the differences in the two approaches and we compare them with the fixed NLO results.

### 15.2 A comparison between NLO, POWHEG and HEJ in dijet production

In order to avoid biasing our event sample, we impose a minimal set of cuts, avoiding symmetric cuts on the jet transverse momenta that would give an unphysical cross section at fixed NLO level [420, 421], due to the presence of unresummed logarithms. Neither the POWHEG or HEJ descriptions suffer from this instability. However, in order to have a sensible fixed NLO cross section to compare with, we impose asymmetric cuts

$$
\begin{equation*}
p_{\mathrm{T}}^{j}>35 \mathrm{GeV}, \quad p_{\mathrm{T}}^{j_{1}}>45 \mathrm{GeV}, \quad\left|y_{j}\right|<4.7, \tag{99}
\end{equation*}
$$

i.e. all jets are required to have a minimum transverse momentum of 35 GeV , and the hardest-jet transverse momentum, $p_{\mathrm{T}}^{j_{1}}$, is required to be greater than 45 GeV . In order to comply with the experimental acceptance, all jets are further required to have an absolute rapidity $\left|y_{j}\right|$ less than 4.7. Jets are defined according to the anti-kt jet algorithm, with radius $R=0.5$. Only events with at least two jets fulfilling Eq. (99) are kept.

In the following, we compare the fixed NLO cross section with the POWHEG first emission results, with the POWHEG results showered by PYTHIA and with the HEJ predictions. The renormalization and factorization scales have been chosen equal to the transverse momentum of the hardest jet in each event, for the HEJ predictions. For the NLO computation (and for computing the POWHEG $\bar{B}$ function), scales are set to the transverse momentum of the so called underlying Born configuration. Scale-uncertainty bands obtained by varying these scales by a factor of two in each direction are shown for the NLO and HEJ results. The scales entering in the evaluation of parton distribution functions and


Fig. 47: The average number of jets as a function of $\Delta y_{\mathrm{fb}}$ (left plot) and of $H_{\mathrm{T}}$ (right plot), as predicted by a fixed NLO calculation, by POWHEG first emission, by POWHEG+PYTHIA and by HEJ. The dotted red lines around the HEJ prediction and the green ones around the NLO result are obtained by varying the renormalization and factorization scales by a factor of two around their central value.
of the strong coupling in the POWHEG Sudakov form factor are instead evaluated with a scale equal to the transverse momentum of the POWHEG hardest emission [417, 386].

In Fig. 47 we plot the average number of jets as a function of the rapidity difference between the most forward and most backward of the jets fulfilling Eq. (99), $\Delta y_{f b}$, on the left-hand side, and as a function of $H_{\mathrm{T}}=\sum_{j} p_{\mathrm{T}}^{j}$ on the right-hand side. The wide-angle resummation implemented in HEJ produces more hard jets than POWHEG and the fixed NLO calculation, as the rapidity separation between the most forward and the most backward jet in the event increases. Both the NLO and the firstemission POWHEG results have at most 3 jets, so that the average number of jets cannot exceed 3 , and give similar results. Additional jets are instead produced by the PYTHIA shower, so that the average number of jets is increased by roughly $20 \%$ with respect to the NLO one, for $\Delta y_{\mathrm{fb}} \approx 7$. For the same separation in rapidity, the HEJ prediction is $45 \%$ larger than the NLO result, with a chance to distinguish among the three approaches.

The dependence of the average number of jets from $H_{\mathrm{T}}$ (right plot) displays a different behaviour: here the showered events have on average more jets than HEJ and the NLO results, as the sum of the transverse momentum of all the final-state jets increases. It is interesting here to comment on the NLO result obtained with the factorization and renormalization scales set to $p_{\mathrm{T}}^{\mathrm{UB}} / 2$, i.e. half of the transverse momentum of the underlying Born configuration. In fact, from the plot, an unphysical behaviour of this quantity emerges: the average number of jets is greater than 3 above $H_{\mathrm{T}} \approx 270 \mathrm{GeV}$. This is due to the fact that the high $H_{\mathrm{T}}$ region is populated mostly by events with 3 jets, two of which have approximately the same high transverse momentum, and the third one is softer with respect to the other two (the cuts in Eq. (99) are always in place). In this configuration, the exclusive two-jet cross section becomes negative, due to incomplete cancellation of the virtual (negative) contribution, now enhanced by a higher value of the strong coupling constant, evaluated at a lower renormalization scale. A more detailed discussion can be found in ref. [422].

As a last example of a kinematic distribution that displays different behaviour if evaluated at NLO or using POWHEG or HEJ, we plot in Fig. 48 the average value of $\cos \left(\pi-\phi_{\mathrm{fb}}\right)$, where $\phi_{\mathrm{fb}}$ is the azimuthal angle between the most forward and backward jets, as a function of their rapidity separation $\Delta y_{\mathrm{fb}}$. For dijet events at tree-level, $\phi_{\mathrm{fb}}=\pi$ since the two jets must be back-to-back, and the average value of the cosine is 1 . Deviation from 1 then indicates the presence of additional emissions, so that


Fig. 48: The average value of $\cos \left(\pi-\phi_{\mathrm{fb}}\right)$ as a function of $\Delta y_{\mathrm{fb}}$, where $\phi_{\mathrm{fb}}$ is the azimuthal angle separation between the most forward and most backward jet. The dotted red and green lines are obtained by varying the renormalization and factorization scales by a factor of 2 in both directions.
this kinematic distribution carries information on the decorrelation between the two jets. This quantity is more inclusive than the average number of jets as it is sensitive also to emissions below the jet $p_{\mathrm{T}}$ cut. The higher radiation activity in POWHEG+PYTHIA and in HEJ, with respect to the fixed NLO and the POWHEG first-emission results, is clearly visible in the figure: the stronger jet activity produced by HEJ at higher rapidity separation (see the left plot of Fig. 47) lowers the average value of the cosine below the POWHEG+PYTHIA result. As expected, the average value predicted by the POWHEG first-emission and the NLO calculation is closer to 1 , since they contain at most one radiated parton.

## Conclusions

In this proceeding, we have discussed the results obtained using a fixed NLO calculation, HEJ and POWHEG+PYTHIA, in the description of three kinematic distributions, selected in order to display more clearly the differences among the three approaches: the average number of jets and azimuthal decorrelation between the most forward and the most backward jet, plotted as a function of the rapidity separation of the most forward and the most backward jet, and the average number of jets plotted as a function of the sum of the transverse momenta of all the jets in the event.

While the limitations of the NLO calculation are clearly visible when we probe regions of the phase space where multi-jet emissions becomes important, the predictions of POWHEG+PYTHIA and HEJ are distinguishable when dealing with the average number of jets as a function rapidity span. Less marked differences are found as a function of Ht , and in the study of the azimuthal decorrelation of the most forward and backward jet.

An experimental analysis of the dijet data, collected at the LHC, should then follow to investigate to which extent our theoretical knowledge for these kinematic distributions is under control.

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## 16. W+JETS PRODUCTION AT THE LHC: A COMPARISON OF PERTURBATIVE TOOLS 30


#### Abstract

In this contribution, we discuss several theoretical predictions for $W$ plus jets production at the LHC, compare the predictions to recent data from the ATLAS collaboration, and examine possible improvements to the theoretical framework.


### 16.1 Motivation

Experimentalists are reliant on a number of tools, at LO and NLO, at parton level and at hadron level, in order to understand both simple and complex final states at the LHC. One of the benchmark processes, for both signals to new physics and for their backgrounds, is the production of $W$ plus jets. In this contribution, we discuss several different predictions for the $W$ plus jets final state, concentrating on the $H_{T}$ distribution. We examine where the predictions agree, and where they disagree and compare the predictions to LHC data. We introduce the idea of NLO 'Exclusive Sums', and discuss the performance of this technique and consider also how LoopSim may be able to improve the predictions. We document the use of ROOT ntuples for $W$ plus jets predictions produced by the BlackHat+Sherpa collaboration, indicating how they can be used to examine the variation of the cross sections with jet size/algorithm, PDFs, and scale choices. We also study the possibility of using the LoopSim method together with BlackHat+Sherpa type ntuples, since this may offer the opportunity to improve on the results from NLO Exclusive Sums.

### 16.2 Theory tools: strengths and weaknesses

NLO is the first order at which the normalization (and sometimes the shape) of LHC cross sections can be realistically calculated. The state of the art is in parton-level programs such as BlackHat+Sherpa, where $W+n$-jet cross sections are available, with $n$ up to 4 at NLO [70, 51, 22] (and soon up to 5 [423]). Of course, such parton-level final states do not allow for the full comparisons to the data allowed by the full parton shower Monte Carlo programs such as Sherpa. NLO matrix elements have been included into parton shower Monte Carlos, but only for relatively simple final states (although we note that the NLO matrix elements for $W+2$ jets [404] and $W+3$ jets [424] have recently been implemented in parton shower Monte Carlo programs).

The Sherpa Monte Carlo program [146, 425] includes the exact LO $W+n$-parton ( $W+n$ jet) matrix elements, with $n$ up to 4 (in this study), using the newer ME\&TS scheme as introduced in Refs. [426, 427, 428] for the addition of states with different jet multiplicities with the correct normalizations. The newer matrix-element plus parton-shower merging scheme improves over the CKKW [429, 430] formalism by allowing for a better interplay between the matrix-element and partonshower descriptions. This in particular required the implementation of truncated showers ('TS'). As before, additional jets are, of course, then produced by the parton shower. Both BlackHat+Sherpa and Sherpa rely on DGLAP-based evolution of gluon emission, on the assumption that the gluon emissions are strongly ordered in transverse momentum. For an alternative prediction, we use the program HEJ [418, 419, 431]. The High Energy Jets (HEJ) framework provides a leading-log resummation of the dominant terms in the limit of large invariant mass between jets. In addition, HEJ contains a merging procedure to ensure tree-level accuracy for final states with two, three or four jets.

[^139]A NLO $n$-jet prediction produces events with with either $n$ or $n+1$ partons. For observables for which higher multiplicities have a significant impact, this limitation can be detrimental. If one has predictions for different multiplicities, one can try to combine them by avoiding double counting by requiring that the $n$-jet prediction is used only to describe $n$-jet events (except for the highest multiplicity where ( $n+1$ )-jets configurations are allowed). This procedure is crude and does not increase the formal accuracy of the prediction which is that of NLO of the smallest multiplicity. The idea is that, in observables where higher multiplicities events dominate, a better prediction might be obtained. This has been denoted as the 'Exclusive Sums' technique. The impact of the Exclusive Sums approach depends on the kinematic variable under consideration. For this contribution, we consider only the $H_{T}$ variable, defined as the sum of the transverse momenta of all of the leptons (including neutrinos) and jets in the event. The impact of the approach is expected to depend on the observable under consideration and it may be more beneficial for variables sensitive to multi-jet radiation, such as $H_{T}$, than for more inclusive variables such as $p_{t, W}$. Comparisons for the latter are left to a study now in progress.

### 16.3 Use of BlackHat+Sherpa ntuples

As has been partially detailed in these proceedings, there have been many advances in the computation of the NLO corrections for multi-parton final states. Often such calculations do not exist in a compact user-friendly form, and other means must be taken to allow experimentalists to have access to the results. The BlackHat+Sherpa collaboration has chosen to make available ROOT tuples that contain all of the parton-level information needed to form flexible predictions. The ROOT ntuple framework is a very efficient way to store such information and the use of ROOT tuples is very familiar to experimentalists.

The ROOT ntuples store the four-vectors for the final state partons, as well as their flavor information. The calculation is originally performed using a specific choice of PDF, $\alpha_{s}\left(m_{Z}\right)$, renormalization scale $\mu_{R}$ and factorization scale $\mu_{F}$, but weight information is also stored in the ntuples that allows each event to be easily re-weighted to any other (reasonable) values for the above parameters. (PDFs are varied through calls to LHAPDF [432].) No jet clustering has been performed on the final state partons; jet reconstruction is left to the user, for any jet algorithm/size for which the correct counter-events are present in the ntuple. For the results presented here, the SISCone [433], $k_{T}$ [361] and anti- $k_{T}$ [341] algorithms, with jet radii $R$ of $0.4,0.5,0.6$ and 0.7 can be used. Each of the above jet algorithms were run and the results stored in SpartyJet ntuples ${ }^{31}$ The SpartyJet tuples were 'friended' with the BlackHat+Sherpa ntuples, allowing the analysis script access to all jet information. Such a flexibility allows for an investigation of the dependence of the physics on the details of the manner in which the partons are combined into jets, in a manner difficult to achieve prior to this.

The four-vector information stored in the BlackHat+Sherpa ntuples is shown in Table 11. Note the variety of entries needed for the re-weighting of the cross section results, especially for the case of the variation of the two scales $\mu_{R}$ and $\mu_{F}$. Information is stored in separate ntuples for the different categories of events, which are typically Born, loop (leading color and sub-leading color), real and subtraction terms. For large $n$, in $W+n$-parton final states, there are many divergences present when two partons become collinear or one parton becomes soft. These divergences are controlled using the traditional Catani-Seymour approach [236], which involves the generation of many counter-events. Many of the events have negative weights; only the sum is guaranteed to be positive-definite. Predictions with reasonable statistical precision may require the sum of billions of events. The resultant tuples may amount to several Terabytes. However, the output can be subdivided into ROOT files of order 5-10 GB, allowing for simultaneous parallel processing of the events over multiple nodes, such as in the Tier3 facility at Michigan State University used for these comparisons.

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### 16.4 BlackHat+Sherpa predictions

We have generated NLO predictions with the BlackHat+Sherpa predictions implementing the cuts used in the 2010 ATLAS $W$ plus jets paper [436]. For completeness, the cuts are reproduced below:

- $p_{T}^{\text {lepton }}>20 \mathrm{GeV}$,
- $\left|\eta^{\text {lepton }}\right|<2.4$,
- $E_{T}^{\text {miss }}>25 \mathrm{GeV}$,
- $m_{T, W}>40 \mathrm{GeV}$,
- $p_{T}^{\text {jet }}>30 \mathrm{GeV}$,
- $\left|y^{\text {jet }}\right|<4.4$,
- $\Delta R^{\text {lepton-jet }}>0.5$.

In Figure 49, we show the NLO BlackHat+Sherpa prediction for the $H_{T}$ distribution for $W+\geq 1$ jets (left) using the anti- $k_{T}$ jet algorithm with $R=0.4$. As the prediction is an inclusive NLO calculation for $W+\geq 1$ jets, there are contributions from both the one-jet and the two-jet final states. Note that as $H_{T}$ increases, the contributions from the $W+2$-jet subprocess also increases. On the right, we again show the $H_{T}$ distribution, but now compute the prediction using the 'Exclusive Sums' technique, adding in the NLO $W+2$-jet information. Now there is a significant contribution at high $H_{T}$ from the $W+3$ -

| branch name | type | notes |
| :---: | :---: | :---: |
| id | I | id of the event. Real events and their associated counter-terms share |
| nparticle | I | number of particles in the final state |
| px | F[nparticle] | array of the x components of the final state particles |
| py | F[nparticle] | array of the $y$ components of the final state particles |
| pz | F[nparticle] | array of the z components of the final state particles |
| E | F[nparticle] | array of the energy components of the final state particles |
| alphas | D | $\alpha_{s}$ value used for this event |
| kf | I | PDG codes of the final state particles |
| weight | D | weight of the event |
| weight2 | D | weight of the event to be used to treat the statistical errors correctly in the real part |
| me_wgt | D | matrix element weight, the same as weight but without pdf factors |
| me_wgt2 | D | matrix element weight, the same as weight2 but without pdf factors |
| x 1 | D | fraction of the hadron momentum carried by the first incoming parton |
| x 2 | D | fraction of the hadron momentum carried by the second incoming parton |
| x1p | D | second momentum fraction used in the integrated real part |
| x2p | D | second momentum fraction used in the integrated real part |
| id1 | I | PDG code of the first incoming parton |
| id2 | I | PDG code of the second incoming parton |
| fac_scale | D | factorization scale used |
| ren_scale | D | renormalization scale used |
| nuwgt | I | number of additional weights |
| usr_wgts | D[nuwgt] | additional weights needed to change the scale |

Table 11: Branches in a BlackHat+Sherpa ROOT file.


Fig. 49: The $W$ plus jets cross section, as a function of $H_{T}$, for the NLO inclusive $W+\geq 1$-jet prediction (left) and for the Exclusive Sums approach, adding in $W+2$-jet production at NLO (right). The cross sections have been evaluated at a central scale of $H_{T} / 2$ and the uncertainty is given by varying the renormalization and factorization scales independently up and down by a factor of 2 , while ensuring that the ratio of the two scales is never larger than a factor of 2 .
jet final state as well. In Figure 50, the $H_{T}$ prediction is shown using the Exclusive Sums approach, adding $1+2+3$ jets at NLO (left) and $1+2+3+4$ jets at NLO (right). It is evident that as $H_{T}$ increases, contributions from higher jet multiplicities that are only present implicitly in a traditional inclusive NLO $W+\geq 1$-jet calculation, become important. The Exclusive Sums $H_{T}$ predictions agree with that for the inclusive NLO $W+\geq 1$-jet calculation at low $H_{T}$, but are larger at higher $H_{T}$, and in better agreement with the ATLAS data (as discussed below).

However, it can also be noticed that the scale dependences for the Exclusive Sums predictions apparently get better when the 2 -jet NLO information is added, but significantly worse when the 3 -jet and 4 -jet information is added. As discussed in the Appendix, the reduction in scale dependence with the addition of the 2-jet NLO terms may be due to the stabilization of the predictions for the $q q \rightarrow W q^{\prime} q$ topologies. Adding the 3 -jet and 4 -jet NLO terms seems to destabilize the predictions. There are missing Sudakov terms needed to properly 'stitch' the different multiplicity samples together; it is hoped that the LoopSim technique may offer one way in supplying those missing terms.

Below in Figure 51, we show the NLO BlackHat+Sherpa predictions for the $H_{T}$ distribution for $W+\geq 2$ jets: the inclusive calculation to the left, the Exclusive Sums result adding $2+3$-jet NLO information in the middle and the Exclusive Sums result adding 2+3+4-jet NLO information to the right. Over the kinematic range covered in these plots, the Exclusive Sums technique adds less to the cross section at high $H_{T}$, although there is still a degradation of the scale dependence.


Fig. 50: The $W$ plus jets cross section, as a function of $H_{T}$, for $W+\geq 1$-jet production using the Exclusive Sums approach, and adding up to 3 jets at NLO (left) and 4 jets at NLO (right). The cross sections have been evaluated at a central scale of $H_{T} / 2$ and the uncertainty is given by varying the renormalization and factorization scales independently up and down by a factor of 2 , while ensuring that the ratio of the two scales is never larger than a factor of 2 .




Fig. 51: The $W$ plus jets cross section, as a function of $H_{T}$, for $W+\geq 2$-jet production using the inclusive NLO production (left) and the Exclusive Sums approach, adding up to 3 jets at NLO (center) and 4 jets at NLO (right). The cross sections have been evaluated at a central scale of $H_{T} / 2$ and the uncertainty is given by varying the renormalization and factorization scales independently up and down by a factor of 2 , while ensuring that the ratio of the two scales is never larger than a factor of 2 .

### 16.5 Towards interfacing BlackHat+Sherpa ntuples with LoopSim

LoopSim is a method to simulate higher order QCD corrections, in particular those beyond NLO. It is expected to work best for processes with large NLO-to-LO $K$-factor, however it was found to be advantageous even in some cases where the $K$-factor is moderate [437]. The method is based on unitarity and its main ingredient is a procedure that takes events from a process with $n+m$ partons in the final state and produces counter-term events with $n+m-1, n+m-2, \ldots, n$ particles, which approximate 1-loop, 2-loop, etc. contributions. In contrast to the Exclusive Sums method, it enables one to introduce (approximate) virtual corrections beyond 1-loop, thus ensuring that the $\alpha_{s} L^{2}$ type terms cancel for all the orders that are included. While we will not show LoopSim results that are directly comparable to the ATLAS data (the samples were generated before those cuts were made public), we will examine below the dependence on the $p_{t, \min }$ choice (which sets the size of $L=\ln O_{t} / p_{t, \min }$ where $O_{t}$ is a transverse observable) and see that it vanishes as $p_{t, \text { min }} \rightarrow 0$.

To distinguish between the exact result at the order $\mathrm{N}^{p} \mathrm{LO}$ and the result with simulated loops we use a notation in which we replace N by $\bar{n}$ for the orders simulated by LoopSim. So for example, $W+1$ jet at $\bar{n} \mathrm{LO}$ has approximate 1 -loop diagrams and is obtained by combining $W+1$ jet at LO with $W+2$ jet at LO where the latter is passed through LoopSim. Similarly $W+1$ jet at $\bar{n}$ NLO has exact 1-loop diagrams but simulated 2-loop contributions (by using $W+2$ jet at NLO as an input to LoopSim).

As argued in the previous section, the BlackHat+Sherpa ntuples allow one to efficiently perform a broad range of analyses. They have however a limitation. In order to reduce the size of stored files, the only partonic events that are recorded for the $W+n$-jet sample are those in which there are at least $n$ jets above a 20 GeV threshold. Since this threshold is below the jet cuts used by ATLAS and CMS, it is adequate for any NLO study of LHC jet cross sections. The situation is slightly more complex if we want to use the BlackHat+Sherpa ntuples to compute predictions beyond NLO using LoopSim. This is because the cut that is present in the $W+2$-jet BlackHat+Sherpa NLO sample eliminates part of the real contribution to the $W+1$-jet phase space at NNLO, for example $W+3$-parton events in which the 3 partons all form part of a single jet, or in which 2 partons form part of one jet, while the third is well separated in angle but below the 20 GeV jet threshold.

Since we plan to use LoopSim interfaced to BlackHat+Sherpa ntuples in our future study of multijet processes, it is important to directly check the effect of the finite generation $p_{t}$ cut, $p_{t, \mathrm{gen}}^{\min }$, on the predictions of the $p_{t}$ and $H_{T}$ distributions. We have performed such a study for $W^{-}+1$ jet generated with MCFM, where we varied a 'parton'- $p_{t}$ generation cut from 1 to $20 \mathrm{GeV}{ }^{32}$ This is not entirely equivalent to the cut in the BlackHat+Sherpa samples (which is applied to the standard jets, not to the partons), but should be adequate from the point of view of estimating the potential order of magnitude of finite generation cuts. The output from MCFM was interfaced to LoopSim which produced the additional loop diagrams. Then, the events were analyzed with the following set of cuts: $\left|y^{\text {lepton }}\right|<2.5, p_{T}^{\text {lepton }}>$ $20 \mathrm{GeV},\left|y^{\mathrm{jet}}\right|<4.5, p_{T}^{\text {jet }}>25 \mathrm{GeV}, m_{T, W}<20 \mathrm{GeV}$, where the anti- $k_{T}$ algorithm with $R=0.4$ was used for clustering.

The results are presented in Figure 52 where the ratios of cross sections obtained with a range of generation cuts are shown as functions of the $p_{t}$ of the leading jet and $H_{T, \text { jets }}$. At NLO, the only artefact we see is for the $p_{t, \text { gen }}^{\min }$ of 20 GeV in the bin below 40 GeV . This is as expected, since a 20 GeV cut on each of two partons can at most affect jets up to 40 GeV (such an artefact would not be present in the BlackHat+Sherpa samples). At $\bar{n} \mathrm{LO}$ and $\bar{n} \mathrm{NLO}$, however, the dependence on $p_{t, \mathrm{gen}}^{\min }$ is extended to a larger range of $p_{t, \text { lead.jet }} / H_{T, \text { jets }}$ and it is visible also for values of $p_{t, \text { gen }}^{\min }<20 \mathrm{GeV}$. However, even if the $p_{t, \text { gen }}^{\min }$ dependence of the $\bar{n} \mathrm{LO}$ and $\bar{n} \mathrm{NLO}$ results is stronger than at NLO, it dies out quickly with increasing $p_{t, \text { lead.jet }} / H_{T, \text { jets }}$ and becomes irrelevant at $\sim 100 \mathrm{GeV}$, depending on the observable and the

[^141]

Fig. 52: Ratios of cross sections from runs with a certain range of $p_{t, g e n}^{\min }$ values taken wrt. the cross section generated with $p_{t, \mathrm{gen}}^{\min }=1 \mathrm{GeV}$ for the distributions of $p_{t}$ of the leading jet (left) and the scalar sum of jets' transverse momenta, $H_{T, \text { jets }}$ (right).
order. This appears to be consistent with the expectation that the effect of the cut should vanish as a power of $p_{t, \text { gen }}^{\min } / p_{t, \text { lead.jet }}$ or $p_{t, \text { gen }}^{\min } / H_{T, \text { jets }}$.

Therefore we conclude, that in spite of the finite generation cut one should be able to trust the results obtained using BlackHat+Sherpa ntuples, above a moderate $p_{t}$ limit, even for more complex analyses such as those involving LoopSim.

### 16.6 Comparisons to data, Sherpa and HEJ predictions

In Figure 53 (left), we compare the ratio of the 2010 ATLAS $W$ plus jets data for the $H_{T}$ distribution for $W+\geq 1$ jets to predictions using the generic NLO calculation for $W+\geq 1$ jet, the Exclusive Sums approach adding up to 4 jets at NLO and the Monte Carlo event generator Sherpa. The agreement between the data and the pure NLO result is rather poor; it improves substantially with the inclusion of the Exclusive sums up to two jets at NLO, with further small improvements coming from higher multiplicities. As a reminder, we previously noted that the scale dependence improved when adding the 2 -jet NLO information, but degraded when adding higher jet multiplicities. The Sherpa prediction slightly overshoots the data for $H_{T}$ in the inclusive $W+1$-jet bin. We however note that the data versus Sherpa $H_{T}$ ratio has been formed based on the absolute normalization as given by the Monte Carlo simulation. Comparing the inclusive 1-jet cross sections, we find a factor of 0.97 between the data and the Sherpa result.

In Figure 53 (right), we compare the ratio of the 2010 ATLAS $W$ plus jets data for the $H_{T}$ distribution for $W+\geq 2$ jets to predictions using the generic NLO calculation for $W+\geq 2$ jet, the Exclusive Sums approach adding up to 4 jets at NLO, and to predictions from HEJ and from Sherpa. As noted previously, there is some increase in the predictions from the Exclusive Sums approach at the highest $H_{T}$ values, but not nearly as much as in the $W+\geq 1$-jet case. These increases go in the direction of closer agreement with the data, but the statistical error does not allow a clear judgement to be made. The Sherpa and HEJ predictions for this ratio are in reasonable agreement with the data but appear to fall off somewhat more rapidly at large $H_{T}$ than either the data or the various BlackHat+Sherpa predictions. Again this partly is the result of relying on the absolutely normalized Monte Carlo predictions, which yield $W+\geq 2$-jet normalization factors of 0.95 or 0.93 between data and Sherpa or HEJ, respectively.


Fig. 53: The ratios of the ATLAS $W+\geq 1$-jet (left) and $W+\geq 2$-jet (right) cross sections, as a function of $H_{T}$, taken wrt. various theory predictions. The absolute normalization has been kept as given by the calculations. The error bars represent the total fractional error (statistical plus systematic added in quadrature) at each point.


Fig. 54: (left) The fraction of the $H_{T}$ cross section for $W+\geq 1$-jet events arising from the $W+\geq 2$-jet, $W+\geq 3$-jet and $W+\geq 4$-jet final states derived from the Exclusive Sums approach, from Sherpa and from HEJ, compared to the 2010 ATLAS data. (right) The ratio of the cross sections for $W+\geq 3$ jets to $W+\geq 2$ jets, as a function of $H_{T}$, using predictions from the Exclusive Sums approach, from Sherpa and from HEJ, compared to the ratio from the 2010 ATLAS data.

In Figure 54 (left), we show the predictions for the fractions of the $H_{T}$ cross section in the inclusive $W+1$-jet bin arising from the inclusive $W+2$-jet, $W+3$-jet and $W+4$-jet final states as obtained from the Exclusive Sums approach and from Sherpa, compared to the 2010 ATLAS data. In Figure 54
(right), we show the ratio of the cross sections for $W+\geq 3$ jets to $W+\geq 2$ jets, as a function of $H_{T}$, again using predictions from the Exclusive Sums approach and from Sherpa but also from HEJ. We again compare to the ratio given by the 2010 ATLAS data. All three predictions agree with each other and with the data over the range considered, despite the big differences in the approaches. There may be an indication of some separation between the predictions at the very highest $H_{T}$ values.

### 16.7 Conclusions, outlook and future studies

The advances achieved over the last few years in calculating NLO corrections for multi-jet final states allow a more serious consideration of the possibility to combine various $n$-jet NLO predictions into an inclusive jet sample. The Exclusive Sums approach discussed in this contribution is a first promising step into this direction. More studies are required to understand the uncertainties related to this procedure. One way of doing so would be to test the stability of the predictions against variation of the jet algorithm and/or parameters of the jet algorithm used to obtain and separate the different NLO predictions for the fixed-multiplicity sets that eventually make up the sum of exclusive $n$-jet contributions. ${ }^{33}$

For the Exclusive Sums approach, outlined here for the case of $W+\geq 1$ jets, contributions are added proportional to $\alpha_{s}^{2}\left(W+1\right.$ jet at NLO), $\alpha_{s}^{3}$ ( $W+2$ jets at NLO), $\alpha_{s}^{4}(W+3$ jets at NLO) and $\alpha_{s}^{5}\left(W+4\right.$ jets at NLO), i.e. this procedure mixes powers of $\alpha_{s}$ and thus is missing essential Sudakov form factors that effectively bring each term to the same power of $\alpha_{s}$. One could imagine accomplishing this by embedding the NLO matrix elements in a parton shower Monte Carlo framework, however the technology for merging different multiplicities of NLO calculations with a parton shower is still under development. Note that at LO the tree-level matrix-element plus parton-shower merging methods (e.g. as implemented in Sherpa) are designed to satisfy this same- $\mathcal{O}\left(\alpha_{s}\right)$ requirement by including the (allorders) leading-log effects to the 'LO Exclusive Sums' exhibiting the LO analog of the Exclusive Sums discussed here. Compared to the matrix-element plus parton-shower merging, we see that the 'NLO Exclusive Sums' technique only accounts for Sudakov effects up to $\mathcal{O}\left(\alpha_{s}\right)$ while it describes each jet bin at full NLO instead of LO accuracy.

Relying on the parton shower Monte Carlo framework is not the only way to go in refining the Exclusive Sums strategy. Alternatively, the LoopSim method can be used to provide approximations to the higher-loop terms missing in the Exclusive Sums approach. As we have seen here, prospects for using it together with BlackHat+Sherpa ntuples seem promising. A detailed comparison of the LoopSim results to LHC data is however beyond the scope of this Les Houches contribution, though we look forward to it being carried out in the near future.

The ATLAS data taken in 2011 is about a factor of 130 times as large as the data taken in 2010 (the only published data for $W$ plus jets so far). This will allow a much further reach in all kinematic variables. To get an idea, we show in Figure 55 the ratio of the predictions from the Exclusive Sums to the respective inclusive NLO predictions for $W+\geq 1,2,3$ jets. At an $H_{T}$ value of 2 TeV , the ratio for $W \geq 1$ jet is of the order of 2 ; the ratio for $W \geq 2$ jets rises to about 1.4. The NLO-to-LO $K$ factor for $W+\geq 1$ jet rises rapidly with increasing $H_{T}$, while the $K$-factor for $W+\geq 2$ jets increases only moderately (because no new subprocesses are being introduced). It will be interesting to see if (a) the additional factor of 2 (for the $W+\geq 1$-jet case) and (b) the additional factor of approximately 1.4 (for the $W+\geq 2$ jet case) lead to better agreement with the data. The LHC data from 2011 (and the higher statistics expected in 2012) will reach these kinematic values and should shed further light on the necessity and the efficacy of this theoretical technique, not only for $W+\geq 1$ jet, but for higher jet multiplicities as well.

[^142]

Fig. 55: The ratio of the predictions obtained from the NLO Exclusive Sums approach to the inclusive NLO predictions for $W \geq 1$ jets, $W \geq 2$ jets and $W \geq 3$ jets. The ' jitter ' is due to the limited BlackHat+Sherpa statistics for these predictions.

## Acknowledgments

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## Appendix: a double logarithmic analysis of the Exclusive Sums method

To help understand the structure of the Exclusive Sums method, it can be useful to consider how it works in a simple double logarithmic approximation. We use $p_{t, \min }$ to represent the minimum $p_{t}$ for the jets in the Exclusive Sums sample, and first study the cross section for $W$ production as a function of $p_{t, W}$ at high $p_{t, W}\left(\gg m_{W}\right)$, considering in particular the terms that go as $\alpha_{s}^{n} L^{2 n}$ where $L=\ln p_{t, W} / p_{t, \min }$. The 0 -jet sample does not contribute at all to non-zero $p_{t, W}$, so the first term comes from the exclusive 1 -jet contribution. If calculated to all orders in the double logarithmic approximation (DLA), it would have the form

$$
\begin{equation*}
\sigma_{1, \operatorname{excl}}^{\mathrm{DLA}}\left(p_{t, W}\right)=\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \exp \left(-\frac{2 C \alpha_{s}}{\pi} L^{2}\right) \tag{100}
\end{equation*}
$$

where $C=2 C_{F}+C_{A}$ for the (dominant) $q g \rightarrow W^{ \pm} q^{\prime}$ scattering process. The $n$ exclusive jet rate would be given by

$$
\begin{equation*}
\sigma_{n, \mathrm{excl}}^{\mathrm{DLA}}\left(p_{t, W}\right)=\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \frac{1}{(n-1)!}\left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)^{n-1} \exp \left(-\frac{2 C \alpha_{s}}{\pi} L^{2}\right) \tag{101}
\end{equation*}
$$

and one sees that the sum over all multiplicities is given by

$$
\begin{equation*}
\sigma\left(p_{t, W}\right)^{\mathrm{DLA}}=\sum_{n=1}^{\infty} \sigma_{n, \mathrm{excl}}^{\mathrm{DLA}}\left(p_{t, W}\right)=\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \tag{102}
\end{equation*}
$$

i.e. in the double logarithmic approximation, there are no corrections to the $p_{t, W}$ distribution at high $p_{t, W}$. Now let us consider what happens if we expand each of the exclusive sums to NLO. For the $n$-jet cross section, we have

$$
\begin{equation*}
\sigma_{n, \mathrm{excl}}^{\mathrm{NLO}(\mathrm{DLA})}\left(p_{t, W}\right) \simeq \sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \frac{1}{(n-1)!}\left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)^{n-1}\left(1-\frac{2 C \alpha_{s}}{\pi} L^{2}\right) \tag{103}
\end{equation*}
$$

Performing the sum over $n$, which corresponds to summing an infinite tower of NLO exclusive jet calculations, leads to

$$
\begin{align*}
\sigma\left(p_{t, W}\right)^{\mathrm{DLA}} & =\sum_{n=1}^{\infty} \sigma_{n, \mathrm{excl}}^{\mathrm{NLO}(\mathrm{DLA})}\left(p_{t, W}\right)  \tag{104a}\\
& =\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \exp \left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)\left(1-\frac{2 C \alpha_{s}}{\pi} L^{2}\right)  \tag{104b}\\
& =\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right)\left(1-\frac{1}{2}\left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)^{2}+\mathcal{O}\left(\alpha_{s}^{3} L^{6}\right)\right) . \tag{104c}
\end{align*}
$$

As long as $L^{2}$ is not large, the difference between this and the correct answer of Eq. 102 is a straightforward NNLO correction, i.e. small. However when $p_{t, W} \gg p_{t, \min }$ the logarithms become large, the $\alpha_{s}^{2} L^{4}$ term can be of order 1 and the Exclusive Sums method may then no longer be a good approximation. A similar analysis can be performed for an exclusive sum truncated at some finite order, as used in our study.

Given the above discussion, one may wonder then if there are any circumstances in which the Exclusive Sums method will bring benefits. For the observable studied in this contribution, $H_{T}$, the key difference with respect to $p_{t, W}$ is that it is subject to a 'giant' $K$-factor at NLO. This phenomenon is associated with 'dijet' topologies in which a soft or collinear $W$ is radiated off the dijet system, leading to a double logarithmic (electroweak) enhancement. In addition these topologies can be created by $q q$ type scattering (whereas the LO process involves only $g q$ or $q \bar{q}^{\prime}$ scattering), leading to further enhancement in $p p$ collisions at large $H_{T}$. Dijet type topologies contribute significantly to the $H_{T}$ distribution, even when the $W$ is soft, because the variable sums all particles' transverse momenta (whereas the softness of the $W$ limits these topologies' contribution to the $p_{t, W}$ distribution).

Because of the giant $K$-factor, for the $H_{T}$ variable the behaviour of the Exclusive Sums method is more subtle than for $p_{t, W}$ : while the $\sigma_{W+2}^{\mathrm{NLO}}$ contributions destabilize the prediction for the $q g \rightarrow W q^{\prime}$ type topologies, they instead stabilize the prediction for the much larger $q q \rightarrow W q^{\prime} q$ topologies (present only at LO in a NLO $W+1$-jet calculation). Going further in the exclusive sum, however, i.e. including $\sigma_{W+3}^{\mathrm{NLO}}$ and $\sigma_{W+4}^{\mathrm{NLO}}$ contributions can however destabilize the predictions for both kinds of topologies. Traces of this behaviour were visible in the numerical studies shown above.

## 17. $W$ PRODUCTION IN ASSOCIATION WITH MULTIPLE JETS AT THE LHC ${ }^{34}$


#### Abstract

We compare the results from four different theoretical predictions for the production of a $W$ boson in association with at least two jets at the Large Hadron Collider. We discuss a possible method for combining next-to-leading order samples with different jet multiplicity from BlackHAT+SHERPA. We then compare these results with the next-to-leading order $W$ plus two jet calculation, the leading order ME\&TS merged approach of SHERPA and the highenergy resummation approach of High EnERGY JETS in an attempt to determine if these approaches can be distinguished at the LHC.


### 17.1 INTRODUCTION

The production of a $W$ boson in association with jets at the Large Hadron Collider (LHC) is an extremely important process. It contributes to three distinct areas of the rich physics program at the LHC. Firstly, it is a key Standard Model signal and therefore important to test our understanding of the Standard Model in the TeV -scale energy range. Secondly, it is an important background in many searches for new physics where, for example, new heavy coloured particles have cascade decay chains. Thirdly, it provides an ideal testing ground for experimental techniques such as a jet veto: what is learned in the relatively well-understood treatment of $W$ plus jets can be directly applied to Higgs searches for example.

It has been observed that the ratio of $W+(n+1)$-jet events to $W+n$-jet events can be substantially larger than one might naïvely expect by considering the $\alpha_{s}$ suppression only. This is especially true in phase-space regions of large four-momenta, such as the high- $H_{T}$ tail, because the available phase space for extra jet emission at the LHC is extremely large. It can therefore compensate for the effect of an additional factor of the strong coupling. This effect is more visible in distributions where additional radiation leads to a significant change in the value of the observable, as is the case for the $H_{T}$ distribution, the scalar sum of the transverse momenta of identified leptons, jets and missing energy. The change will be more moderate in an observable like $H_{T, 2}$, whose definition differs from that of $H_{T}$ by truncating the jet sum to include only the two hardest jets in the event. To make an impact here requires the radiation to lead to an additional jet with transverse momentum as large as that of the second hardest jet, not only larger than the jet $p_{T}$ threshold. The effects will also be smaller in more inclusive variables like the transverse momentum of the $W$ boson, $p_{T, W}$, or the leading jet, $p_{T, j_{1}}$.

There are a number of different theoretical approaches to describing the emission of large numbers of jets. In order to probe to what extent the differences in these will be accessible at the LHC, we will compare, in this study, the predictions for the jet activity in inclusive $W(\rightarrow e \nu)+2$-jet production from (a) BLACKHAT+SHERPA $(B H S)$ [70, 51, 22], (b) combined $B H S$ samples (to be described below), (c) Sherpa [146, 425] run in ME\&TS mode (S-MEPS) [426, 427, 428] and (d) High Energy Jets (HEJ), an all-order resummation of wide-angle radiation [418, 419, 438].

The current state-of-the-art next-to-leading order (NLO) predictions for $W$ production in association with jets are those of $B H S$, which have been calculated up to $W$ plus four jets with a leading-colour approximation for the virtual part [22], and up to $W$ plus three jets with a full color treatment [70, 51]. In this study, we consider the inclusive $W+2$-jet prediction at NLO accuracy, and further, discuss and show predictions from an inclusive sample where $W+2,3,4$-jet events generated by $B H S$ are combined in a simple manner, nevertheless without introducing any double counting of phase-space regions.

The $S$-MEPS predictions are obtained from merging at leading order (LO) tree-level Matrix Elements for $W+0, \ldots, n$-parton final states with (Truncated) parton Showers (hence the name ME\&TS) preserving the leading logarithmic accuracy to which soft and collinear multiple emissions are described by the parton shower. The newer ME\&TS merging scheme was introduced in Ref. [426] and optimised

[^143]as documented in Refs. [427, 428] to improve over the original SHERPA implementation based on the CKKW approach [429, 430]. ME\&TS guarantees a better matching regarding the usage of scales as occurring in the evaluation of the matrix elements and those scales driving parton showering. The $S$-MEPS sample used in our study was generated by including $W(\rightarrow e \nu)$ production matrix elements with up to five extra partons (massless quarks, $u, d, s, c, b$, and gluons).

The HEJ framework is a resummation of the leading logarithmic terms occurrung in pure, or $W$, $Z$ or $H$ plus, multi-jet production in the limit of large invariant mass between each pair of jets, to all orders in $\alpha_{s}$. This is then matched to tree-level accuracy for final states with two, three or four jets. In principle, the HEJ framework can be merged with a parton shower to add the collinear pieces which are not included in the HEJ description (HEJ does include soft emissions down to around 2 GeV ). First steps in this direction for pure jet production were taken in [431]. Here, the HEJ predictions are calculated at the parton level.

In the 17.2 section, we will elaborate on the method (b) for combining NLO samples of different jet multiplicities. Then, in the 17.3 section, we will first show explicit results of the sizable impact of large multiplicity events by comparing predictions from the combined BHS sample and the S-MEPS merged sample. Secondly, we will study variables chosen to probe the differences in the treatment of the QCD radiation. We will show and compare the predictions for all four descriptions mentioned above focusing on the following observables:

- the average number of jets as a function of $H_{T}=\sum_{i} p_{T, j_{i}}+p_{T, e}+p_{T, \nu}$ and $\Delta y$, the rapidity difference between the most forward and most backward jets, and also
- the ratio of the inclusive 3-jet rate to the inclusive 2-jet rate as a function of $H_{T}$ and $\Delta y 35$

We will then discuss the areas of agreement and difference that we find, before we finally conclude in the 17.4 section.

### 17.2 NLO EXCLUSIVE SUMS

An NLO $n$-jet prediction contains events with $n$ or $n+1$ partons. For observables for which higher multiplicites have a significant impact, this limitation can be detrimental. If one has predictions for different multiplicities ( $m, m+1, \ldots, M$ ), one can try to combine them by avoiding double counting by requiring that the $n$-jet prediction is used only to describe $n$-jet events (except for the highest multiplicity where ( $n+1$ )-jets configurations are allowed). The total cross section can be rewritten as a decomposition based on exclusive (exc) and inclusive (inc) jet bins:

$$
\begin{equation*}
\sigma^{\mathrm{tot}} \equiv \sigma_{m}^{\mathrm{inc}}=\sum_{n=m}^{M-1} \sigma_{n}^{\mathrm{exc}}+\sigma_{M}^{\mathrm{inc}} \tag{105}
\end{equation*}
$$

The exclusive-sums procedure describes each jet bin at NLO accuracy, i.e. at $\mathcal{O}\left(\alpha_{s}^{n+1}\right)$, or, alternatively, only the $(M+1)$-th (inclusive) jet bin is predicted with LO precision. We hence note that the combination of the terms shown in Eq. 105) occurs at different orders of the strong coupling. Furthermore, the definition of an exclusive $n$-jet sample requires a detailed treatment of jet vetoing. For these reasons, the simple combination procedure is crude and does not increase the formal accuracy of the prediction, which is that of NLO of the smallest multiplicity. However, one can hope that the procedure will lead to a better prediction in observables where higher multiplicity events dominate.

More studies are required to understand the uncertainties related to this procedure. One way of doing so would be to vary the jet algorithm and/or parameters of the jet algorithm used to separate the different NLO predictions into fixed multiplicities sets and test the stability of the prediction ${ }^{36}$ This is left to a future study.

[^144]\[

$$
\begin{array}{ll}
\left|\eta_{e}\right|<2.5 & p_{T, e}>20 \mathrm{GeV} \\
M_{\perp, W}>20 \mathrm{GeV} & p_{T, \nu}>20 \mathrm{GeV} \\
\left|\eta_{j}\right|<4.5 & p_{T, j}>25 \mathrm{GeV}
\end{array}
$$
\]

Table 12: Summary of the cuts applied in the analysis.


Fig. 56: The average number of jets as a function of $p_{T, W}$ (left) and $p_{T, j_{1}}$ (right). The $p_{T, W}$ plot shows the $B H S$ exclusive sums prediction, while the $p_{T, j_{1}}$ plot is obtained from $S$-MEPS.

### 17.3 RESULTS OF THE COMPARISON

In this section, we compare the results of different theoretical descriptions for $W+n$-jets production at the LHC. The number $n$ can take values from 2 and above, as we will mostly consider inclusive samples. The four descriptions, which we will compare here in more detail, are

- the $B H S$ calculation of $W+2$-jets at NLO,
- the combined sample of $W+2,3,4$-jet events at NLO from $B H S$, as described in the 17.2 section,
- the $S$-MEPS merged $W+n$-jets sample using LO tree-level matrix elements up to $n=5$, and
- the approach of HEJ.

Throughout this study, we will consider inclusive samples of $W^{-}$boson production in association with at least two hard jets identified by the anti- $k_{T}$ jet algorithm using $R=0.4$. The jets are required to have $p_{T, j}>25 \mathrm{GeV}$. We look only in the $W^{-} \rightarrow e^{-} \bar{\nu}_{e}$ decay channel and use the cuts given in Tab. 12 where $M_{\perp, W}$ is defined as $M_{\perp, W}=\sqrt{\left(\left|\vec{p}_{T, e}\right|+\left|\vec{p}_{T, \nu}\right|\right)^{2}-\left(\vec{p}_{T, e}+\vec{p}_{T, \nu}\right)^{2}}$.

The HEJ predictions use the geometric mean of the jet transverse momenta to determine the renormalisation and factorisation scale, i.e. $\left(\prod p_{T, j}\right)^{1 / n}$. This central choice will be varied by a factor of two in either direction to provide an envelope (marked by dotted lines in the corresponding figures) around the HEJ default prediction. The BHS predictions instead use $\hat{H}_{T}^{\prime} / 2$ as the NLO calculation becomes unstable for a scale which is too low. In the $S$-MEPS calculation, scales are chosen according to the default prescription given by ME\&TS [426].

The variables $H_{T, 2}, p_{T, W}$ and $p_{T, j_{1}}$ are less sensitive to the presence of additional radiation than $H_{T}$, as discussed in the introduction. The plots, which we present in Figs. 56 and 57 address the alternative question: given a particular value of $H_{T}, H_{T, 2}$ etc. how many jets are typically found in the event?

Figs. 56 and 57 show the stacked results for the average number of jets as a function of $p_{T, W}, p_{T, j_{1}}$, $H_{T}$ and $H_{T, 2}$ visualising the contributions from each exclusive 2,3,4-jet sample and the inclusive 5 -jet


Fig. 57: The contribution from different multiplicities to the average number of jets as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the BHS exclusive sums prediction, while the lower ones are extracted from S-MEPS.
sample. The left (right) plot in Fig. 56 and the upper (lower) rows of plots in Fig. 57 depict the results as obtained from the combined BHS sample (the $S$-MEPS sample). In all cases the different colours correspond to the terms in the numerator of the formula for the average number of jets,

$$
\begin{equation*}
\langle N\rangle_{5}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{106}
\end{equation*}
$$

where blue, green, red and magenta stand for $i=2,3,4$ and $i=5$, respectively. The subscript to $\langle N\rangle$ clarifies that we truncate the determination of the average after the fifth jet bin, noting that $\langle N\rangle_{k} \rightarrow\langle N\rangle$ for a sufficiently large number of jet bins. This makes no difference for the BHS predictions employed here since the jet multiplicity de facto is limited to five, but it does for the $S$-MEPS and HEJ computations where events with $i>5$ jets do occur. We have defined $n_{k}^{\text {exc } / \mathrm{inc}}=d \sigma_{k}^{\text {exc } / \mathrm{inc}} / d O$ where $O$ denotes an observable like $H_{T}$, or $\Delta y$ presented later on. Note that in Fig. 57 the 5 -jet part contributes to the average number of jets with a factor of 5 , while the 2 -jet part, for example, contributes with a factor of 2 only.

The layout of Fig. 58 (including the colour coding) is the same as before: here, we however display, wrt. $n_{2}^{\text {inc }}$, the relative fractions of the different multiplicities corresponding to the terms in the denominator of Eq. (106). In other words, in Fig. 58 we consider the partitioning of

$$
\begin{equation*}
1=\frac{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{107}
\end{equation*}
$$



Fig. 58: The fraction of the total rate from different multiplicities as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the $B H S$ exclusive sums prediction, while the lower ones are extracted from $S$-MEPS.

Although there is just a $30 \%$ fraction of inclusive 5 -jet events to the total cross section, we observe that their contribution to the build-up of $\langle N\rangle\left(H_{T}\right)$ for very large $H_{T}$ gets close to $50 \%$. Also, for an $H_{T} \sim$ 500 GeV , the average number of jets is composed evenly between the 2,3 -jet and 4,5 -jet contributions, while the relative fraction of the 2,3 -jet events is nearly $70 \%$. This emphasizes the dominance of multijet events in forming large $H_{T}$ values. It also can be seen that for medium $H_{T}$ values, $400<H_{T}<$ 700 GeV , all the multiplicities give roughly the same contribution to the variable $\langle N\rangle\left(H_{T}\right)$, while for low $H_{T}$, the average is primarily described by 2-jet events.

Going clockwise through Figs. 56 and 57 we see that the average number of jets is indeed sensitive to higher multiplicities when considered as a function of $p_{T, W}, p_{T, j_{1}}$ and $H_{T, 2}$, but in all these cases this happens to a lesser extent as if considered as a function of $H_{T}$. As expected, the dependence is mildest for $p_{T, W}$, the most inclusive observable studied here. We also observe that the jet-bin decomposition of $p_{T, j_{1}}$ and $H_{T, 2}$ turns out very similar. Most strikingly we note the increase in the contribution from the highest multiplicity events, the ones containing more or at least five jets. For $H_{T, 2}$, we furthermore display to the right of Fig. 58 the relative fractions as done in the $H_{T}$ case. Even for largest $H_{T, 2}$ values, the fraction arising from 2,3 -jet events remains close to $65 \%$ stressing once more the lower sensitivity of $H_{T, 2}$ versus $H_{T}$ regarding multiple jet production.

Finally, we compare the plots from the combined BHS samples in all figures to the corresponding ones generated with the $S$-MEPS sample. Interestingly, the outcome looks very similar although ME\&TS handles the single terms in Eq. (105) rather differently. They are calculated at least at leading (soft/collinear) logarithmic accuracy improved by LO $n$-jet effects. Presumably, for the exclusive jet bins, this description (which allows a better treatment of jet vetoes) is not too far off the exclusive sums


Fig. 59: Average number of jets as a function of $H_{T}$ (left) and $\Delta y$ (right) in two BHS descriptions, from $H E J$ and from $S$-MEPS, the latter using the $\langle N\rangle_{7}$ definition. The bands shown with dotted lines for the HEJ prediction are a result of varying the scale by a factor of 2 in each direction.
approach, since the unresolved $\mathcal{O}\left(\alpha_{s}\right)$ corrections are also present in the Sudakov form factors applied in the ME\&TS approach. Also, the combined BHS samples as well as the $S$-MEPS sample use the same tree-level matrix elements, namely up to $W+5$-parton matrix elements. Clearly, it has to be studied further whether this similarity in the results is a coincidence or not.

It is clear that the impact of the higher multiplicity samples is significant throughout, especially in the high $H_{T}$ tail. This is precisely the region, which would be probed for signs of new physics, and therefore it is essential that we fully understand our theoretical descriptions in this region. This is the subject of the remainder of this contribution, where we compare all four different methods of modelling hard QCD radiation in inclusive $W+2$-jet events.

The left plot of Fig. 59 shows the final comparison plot between the exclusive sums and inclusive 2-jet $B H S$ results as well as the $H E J$ and $S-M E P S$ predictions for the average number of jets as a function of $H_{T}$. The differences in the descriptions are significantly larger than the scale uncertainty band on the $H E J$ prediction. For the $W+2$-jet NLO result, the number of jets rises to 2.6 already at $H_{T}=500 \mathrm{GeV}$ but that levels off significantly below the $S-M E P S$, exclusive $B H S$ sum and $H E J$ results. The $H E J$ results level off at a higher value of about 3.0 , starting to clearly disagree with the exclusive sums and $S$-MEPS predictions above 500 GeV , from where those two curves keep rising to a final level of around 3.7 to 4.0. The $S$-MEPS comes in highest at largest $H_{T}$, where $\langle N\rangle_{7}$ is shown, cf. Eq. (106), in order to determine the average number of jets for this $S$-MEPS result. The reason for giving slightly higher $\langle N\rangle$ than the exclusive sums lies in the contribution of additional parton-shower jets present in the $S$-MEPS calculation and more accurately accounted for by the use of the $\langle N\rangle_{7}$ definition as compared to the earlier result based on $\langle N\rangle_{5}$ presented in Fig. 57 to the lower left.

In the right panel of Fig. 59, we have plotted the average number of jets as a function of the rapidity span, $\Delta y$, instead of $H_{T}$ as before. Again the differences are larger than the scale variation shown on the HEJ result, but the ordering is different to that of the left plot of Fig. 59. All four descriptions increase linearly with $\Delta y$ but the gradient is steepest for the HEJ predictions where the average rises above 3.0 for $\Delta y$ values as large as 6.0. The BHS exclusive sum result is consistently below this, reaching about 2.8 at $\Delta y=6.0$, and agrees pretty well with the $S$-MEPS result based on $\langle N\rangle_{7}$. The NLO $W+2$-jet prediction given by $B H S$ is lower still, between 2.4 and 2.5 for $\Delta y \sim 5.0$.

It may seem surprising that on the plot on the left-hand side the exclusive sums and S-MEPS lie higher for most of the distribution whereas on the right-hand side these approaches as well as $H E J$ give predicitions that are commensurate. The region of high $H_{T}$ and that of high $\Delta y$ however are largely distinct as it is very expensive to have both a large rapidity and large $p_{T}$ for the jets. Also while radiating


Fig. 60: The ratio of the inclusive 3 -jet and 2 -jet rates in the inclusive $W+2$-jet NLO and exclusive sum description of $B H S$ as well as in the $S$-MEPS and $H E J$ approaches as a function of $H_{T}$ (left) and $\Delta y$ (right). Again, the dotted lines indicate the uncertainty band from varying the scale in $H E J$ by a factor of 2 in each direction.
an additional jet automatically moves an event towards the higher $H_{T}$ direction, radiating an additional jet tends to not change the rapidity difference. So, we expect the higher multiplicies to have a smaller effect on the average number of jets as a function of $\Delta y$ compared to as a function of $H_{T}$. This is indeed the case in Fig. 59.

Lastly, in Fig. 60 we plot the ratio of the inclusive 3 -jet to the inclusive 2 -jet rate as a function of $H_{T}$ (left) and $\Delta y$ (right), again for all four descriptions used here. The predicted $\left(d \sigma_{3}^{\text {inc }} / d H_{T}\right) /\left(d \sigma_{2}^{\text {inc }} / d H_{T}\right)$ all agree very well below 400 GeV . The fixed order $B H S$ result for $W+2$ jets is highest for large $H_{T}$, however is known to become unreliable here, since the probability that an inclusive 2 -jet event is at least a 3 -jet event turns too large, being in conflict with the expected behaviour of an $\mathcal{O}\left(\alpha_{s}\right)$ correction. The BHS exclusive sums, the S-MEPS and the HEJ results, in this order, level off considerably lower with the HEJ fraction staying below $60 \%$ to $70 \%$, which leaves the other predictions again above the $H E J$ uncertainty envelope. In contrast, when the same ratio of jet rates is plotted against $\Delta y$, the $H E J$ prediction is consistently higher throughout. This again emphasises that differences in the descriptions come to light in different kinematic regions. However, in both cases here the magnitude of the differences is relatively small and would be rather difficult to distinguish in present experimental data.

### 17.4 CONCLUSIONS

We have compared a number of theoretical descriptions of $W^{-}$production in association with at least two jets. After outlining one possible method of combining NLO calculations of different multiplicities, we compared this with a pure NLO calculation of $W+2$-jets production obtained by BLACKHAT+SHERPA, a sample of leading-order events merged using the ME\&TS method of SHERPA, and the high-energy resummation of the HEJ framework.

We studied the average number of jets and the ratio of the 3 -jet and 2 -jet inclusive cross sections as a function of $\Delta y$ and of $H_{T}$. We find, with these simple cuts, some clear differences in the predictions when we study the average number of jets as a function of both $\Delta y$ and $H_{T}$. Smaller differences, which would be more difficult to disentangle experimentally, are found when we study the ratio of inclusive rates.

It would be very valuable to have an experimental study, which probed the average number of jets in $W$ production in association with at least two jets, to test our different descriptions of these important Standard Model processes.

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## 18. UNCERTAINTIES IN THE SIMULATION OF $W+$ JETS - A CASE STUDY 37


#### Abstract

In this contribution, uncertainties in the simulation of a large variety of observables related to the production of $W$ in association with jets at the LHC and the Tevatron are discussed. This work aims to - serve as a compendium of currently publicly accessible tools in addition to the ones presented in a previous publication [439] with a similar topic, and to compare their results; - discuss the origin and generic size of various uncertainties in the simulation of perturbative and non-perturbative aspects of this process; - trace the interplay of these uncertainties in various stages of the full event simulation; - hint at those uncertainties in each of the various tools considered here which the respective authors find relevant; - guide their users in how to assess the related uncertainties in a way the authors recommend.


### 18.1 Introduction

The production of $W$-bosons in association with jets constitutes an important process at the Tevatron and the LHC, for a variety of reasons. First of all, it represents a major background to Standard Model signatures such as top-pair and single-top production, and it also plays a role in searches for the Higgs boson in the Standard Model. Furthermore, this reaction, together with the fairly similar channel of $Z$ production in association with jets, provides one of the most important backgrounds in those searches for new physics where large missing transverse energy and high jet multiplicities characterise the respective signal. Thirdly, this process has become a standard reaction for QCD studies at hadron colliders, ranging from the validation of simulation tools for multijet signatures to measurements related to multiple parton scattering. Finally, this process also provides one of the main testbeds for novel techniques in the automation of higher-order QCD corrections and their matching or merging with subsequent parton showers in the framework of event generators.

In the spirit of this last point, providing a testbed for the combination of fixed order calculations with the parton shower, this process has been analysed in quite some depth in [439] about five years ago. A number of reasons provide motivation to update and extend this previous study, namely

- the LHC being up and running and starting to provide highly precise data such that a proper treatment of uncertainties becomes an important issue;
- major improvements in the ability to calculate higher-order corrections including up to four jets in the final state accompanying the $W$ bosons [51, 117, 22];
- the advent of such next-to leading order calculations - albeit for lower final state multiplicities fully matched to the parton shower [440, 404, 424];
- an improved understanding of the leading order merging prescription for towers of multijet multiplicities with the parton shower [426, 441];

[^145]- the combination of matching and merging methods [442, 443];
- and new methods to simulate multijet topologies based on the high-energy limit [64].

Therefore this study aims at being a first step towards a more complete update of [439], with a shift in focus towards a discussion of theoretical uncertainties in different approximations, including perturbative and non-perturbative effects. Apart from tracing the origin and determining the generic size of various uncertainties in the theoretical description of various observables related to this process, also the interplay of them at various stages of the simulation, from the matrix element to the hadron level will be discussed. Consequently, the most important causes for theory uncertainties in various tools are highlighted. Therefore, one of the more practically relevant goals is to also provide methods to reliably and robustly estimate such uncertainties for the various tools used in this study, as recommended by authors or users.

The outline is as follows: After briefly presenting the various tools included in this study and discussing the way they have been used here in Sec. 18.2 , example results for them will be presented individually, tool by tool in Sec. 18.3 . In Sec. 18.4 these results are compared in order to see and quantify relative differences. In this endeavour, experimental results have not yet been included. We reserve this comparison with relevant data for a later, full-fledged analysis, which will hopefully include even more tools.

### 18.2 Codes

In this work a variety of different codes has been employed, which allow to study the process at various different stages:

1. Fixed order matrix elements:

By now, the description of $W$ boson production in association with jets is possible for up to 4 additional jets at NLO. Here, results from two NLO codes, GoSAM+SHERPA [12, 425, 146] and BLACKHAT+SHERPA [70, 51, 22], which are either publicly available or provide publicly available event files, are presented. The corresponding results therefore are on the matrix element level.
2. All-order resummed matrix elements:

Approximations to the partonic matrix elements for the processes of $n$-jet production, and $W, Z, H+n$-jets, $n \geq 2$, was recently calculated to any multiplicity, and including all-order resummations for the leading virtual corrections. The all-order scheme [418, 419], implemented in the HEJ [64] code, becomes exact in the limit of large invariant mass between each parton (the MRK limit of BFKL). The resummation scheme is merged with LO matrix elements (much like in MEPS, see later). The resummation of HEJ can also be interfaced to a parton shower [431]; the results presented here, however, are on the matrix element level. It should also be stressed that due to the nature of the approximation of HEJ, the simulation here are relevant for the production of at least two jets in addition to the $W$ boson.
3. Parton showers:

The pure parton shower code relies on the collinear approximation to produce additional jets. By using a matrix element reweighting, however, in the process of $W$ production, typically one additional jet can correctly be described. For this simulation, PYTHIA8 [348] has been used here, with results available on the parton shower level, hadron level and hadron level including UE.
4. LO matrix elements merged with the parton shower (MEPS):

By now, the use of towers of multijet matrix elements with increasing multiplicity merged to the parton shower following ideas presented in [444, 429, 445, 430] is common practise in the experimental collaborations. In fact, a first comparison of different codes and implementation has been presented a while ago [439]. Here, three implementations of these ideas are included, namely the ones in MADGRAPH+PYTHIA [165, 446, 163, 191, 400], PYTHIA8+ME [441] and SHERPA [146]. Here results are available on all levels matrix element level, parton shower level, hadron level,
hadron level including UE, and hadron level including UE and QED final state radiation in different combinations of codes.
5. NLO matrix elements matched to the parton shower ( $\mathrm{NLO} \otimes \mathrm{PS}$ and MENLOPS):

In principle two methods by now have been proposed and fully implemented which consistently match full NLO calculations to the parton shower, namely Mc@NLO [401] and Powheg [416, 417]. Here the latter is being used, with its implementation in the Powheg Box [13], and interfaced to the PYthia [400] parton shower in its $k_{T}$-ordered version [447]. In addition, a combination of such matching with the merging methods described in the previous point is available [442, 443], ranging under the name MENLOPS. In this paper we use an implementation of such methods provided in the SHERPA framework. In both cases, results are available on all levels matrix element level, parton shower level, hadron level, and hadron level including UE.

### 18.21 BLACKHAT + SHERPA

The NLO predictions are obtained by combining BLACKHAT [4] for the virtual part and SHERPA [147, 448] for the real part. It is currently possible to obtain predictions at NLO for a $W$-boson in combination with up to four jets [70, 51, 22].

The plots have been produced by re-analysing large event files produced by the combination of BLACKHAT and SHERPA. These files contain particle four-momenta as well as the coefficients of all scale dependent functions, including the PDFs so that it makes it possible to easily change factorisation and renormalisation scales as well as the PDF set.

We used a common factorisation and renormalisation scale $\mu_{F}=\mu_{R}=\hat{H}_{T}^{\prime} / 2$ with $\hat{H}_{T}^{\prime}=$ $\sum_{j} p_{T}^{j}+E_{T}^{W}$ where the sum runs over all jets and $E_{T}^{W}=\sqrt{M_{W}^{2}+\left(p_{T}^{W}\right)^{2}}$.

Estimation of uncertainties The estimation of the uncertainties for the NLO calculation obtained with BLACKHAT+SHERPA is obtained by combining in quadrature the pdf uncertainties obtained using the pdf error set and the uncertainties obtained by varying the factorisation and renormalisation scales simultaneously by factors of $1 / 2$ and 2 . To this error we also add in quadrature the integration error estimate. Another way of estimating the uncertainties due to the choice of scales is to compare predictions obtained using different choice of basis scales, but this has not been done for this study.

We used the CTEQ6.6 PDF set. The value of $\alpha_{s}$ used for this calculation has also been taken as that provided with this PDF set. The PDF uncertainties are estimated using the hessian method and PDF 'error' set provided with the CTEQ6.6 PDF set.

### 18.22 GOSAM + SHERPA

GOSAM [12] is a new framework which allows the automated computation of one-loop scattering amplitudes for multi-particle processes. The one-loop scattering amplitudes are generated in terms of algebraic $d$-dimensional unintegrated amplitudes, which are obtained via Feynman diagrams. This allows to perform symbolic manipulations of the expressions prior any numerical step. For the reduction, the program offers the possibility to use either a $d$-dimensional extension of the OPP method [121, 122, 119], as implemented in SAMURAI [6], or tensor reduction as implemented in golem95 [130, 131] interfaced through tensorial reconstruction at the integrand level [124].

The GoSAM framework can be used to calculate one-loop corrections within both QCD and electroweak theory. Beyond the Standard Model theories can be interfaced using FeynRules [137] or LanHEP [136].

To produce results for a certain process specified by the user, the program must be fed with an "input card" with the details of the process. Alternatively, when interfacing the program with a Monte

Carlo (MC) event generator which supports the Binoth-Les-Houches-Accord (BLHA) interface [145], the specific order file produced by the MC event generator can be passed to GoSAM.

The analysis presented here was performed using this latter generation mode and SHERPA [425] 146] was chosen as MC event generator. SHERPA provides therefore the matrix elements for the production of $W$ and exactly one jet at the Born-level and the NLO real corrections to it, together with the needed subtraction terms and their integrated counter-parts. GOSAM provides the NLO virtual-part. The generation of the code follows the standards of the BLHA-interface [145]. During the first call of Sherpa an "order file" is written by the MC program. This file is read-in by GOSAM to produce the code for the one-loop evaluation of needed process. If this happens successfully, a contract file with information on the different possible subprocesses is produced by GoSAM and can be later read by the MC generator to recognize the numbering of the different partonic subprocesses. At running time all information between GoSAM and SHERPA is also passed using the BLHA-interface standards.

The steering of the event generation and the analysis interface with RIVET [360] is done using SHERPA cards. Each curve in the analysis consists of 100 combined runs of 50 million events. The renormalisation and factorisation scales are set according to the choice made for this analysis in Les Houches to

$$
\mu_{F}=\mu_{R}=\hat{H}_{T}^{\prime} / 2
$$

where $\hat{H}_{T}^{\prime}$ is defined in the previous section.

Estimate of uncertainties The estimation of the uncertainties for the NLO calculation obtained with GoSAM+SHERPA is done combining in quadrature the PDF uncertainties with the uncertainty coming from the separate variation of factorisation and renormalisation scale by factors of $1 / 2$ and 2 . Ideally also the integration error should be added in quadrature to the previous estimate, however the MC integration error obtained with RIVET at NLO is not reliable because of the incapacity of RIVET to take into account properly the correlation between real and subtraction events. For this reason and because of the very high statistics of the MC sample, the MC integration error is neglected. To assess the PDF uncertainty we compute the envelope of the results obtained using the three different PDF sets CT10 [255], used as nominal set, MSTW08 [262] and NNPDF2.1 [312]. The total scale uncertainty is determined by adding in quadrature the factorisation and renormalisation scale uncertainties. Each of them is found by computing the maximum between the nominal value and the up and down variations.

### 18.23 HEJ

The High Energy Jets (HEJ) framework [418, 419] provides an alternative description of collider events to the standard fixed order calculations (possibly interfaced to a parton shower). Instead, HEJ uses approximations to the hard scattering matrix element to all orders in $\alpha_{s}$ which become exact in the High Energy limit. The approximation results in sufficiently simple matrix elements, that these can be explicitly regulated, integrated and summed over any (relevant) multiplicity. This results in an explicit all-order resummation of the dominant contributions from wide-angle QCD radiation.

The building blocks of the HEJ framework ensure the correct leading logarithmic behaviour in the Multi-Regge Kinematic limit (aka. the High Energy Limit) of large invariant mass between all partons, for both the real and virtual corrections. The resummed $n$-jet rate is then further matched to tree-level accuracy for events with up to and including four jets, using a merging procedure for the soft radiation.

This procedure has so far been applied to the production of jets [64], $W$ plus jets [449], $Z$ plus jets and Higgs boson plus jets and has currently been implemented in a fully flexible Monte Carlo for the first two of these processes. The implementation integrates explicitly over any number of QCD emissions from a $(W, Z, H+)$ dijet system, and hence produces event samples for processes with two jets or more. Note that one has access to the momenta of all final state particles for every event and it is therefore extremely simple to restrict to a subset of the events if required, e.g. 3-jet exclusive events.

The HEJ resummation includes emissions at large transverse momentum which are increasingly important as the centre-of-mass energy of particle collisions increases. HEJ is currently the only available flexible Monte Carlo generator to obtain leading logarithmic accuracy in the limit of large invariant mass between emissions. However, the HEJ framework does not include any systematic resummation in the collinear limit. This is included in a parton shower, but a careful merging procedure is required to link one with HEJ, as there is significant overlap between the soft emissions included in each approach; the first steps in this direction have been taken for jet production [431] and are ongoing. In the current study though, only parton level predictions are given.

Estimate of Uncertainty The HEJ framework does not contain any tunable parameters other than the choice of renormalisation and factorisation scale (just like any fixed order calculation). In this study, in common with other approaches, we choose both of these to be given by the geometric mean of the transverse momentum of the jets:

$$
\begin{equation*}
\mu_{R}=\mu_{F}=\left(\prod_{j=1}^{n} p_{T}^{j}\right)^{1 / n} \tag{18.2.1}
\end{equation*}
$$

where the jets are defined according to the relevant cuts in each analysis. This is however only an arbitrary choice, as the framework admits any choice for the scale, including $H_{T}, p_{T}$ of the hardest jet and a fixed scale. For a given scale, $\alpha_{s}$ is evaluated according to the relevant PDF.

In common with standard convention, we calculate the scale variation by changing this scale by a factor of two in both directions. In principle, one could also include the PDF uncertainty, but this is not done in this study (as the scale uncertainty dominates). As described above, HEJ contains matching to tree-level accuracy for up to four jets. However, unlike the merging procedure in a showered sample, the merging scale here is not a free parameter. There is only one rational choice for the merging scale: the minimum $p_{T}$ of a jet in the relevant analysis. However, in an inclusive sample with at least two jets, one could use as a further estimator of uncertainty the variation obtained when matching to three and four jet LO matrix elements. This procedure will be studied in detail in Ref. [449], but in the present study, we quote the uncertainty only from the scale variation.

### 18.24 MADGRAPH + PYTHIA

MADGRAPH [165, 446, 163, 191] is a general purpose leading order matrix element (ME) generator, with a broad variety of models available and easily extensible thanks to its modular structure. The event generation is performed by the MADEVENT component, a tool implementing the Single Diagram Enhanced algorithm for multi-channel phase space integration. When a user provided process is specified, MADGRAPH automatically generates the amplitudes for all the relevant subprocesses and produces the mappings for the integration over the phase space. This process-dependent information is then used by MADEVENT, where the process specific code generated allows the user to calculate cross sections and to produce unweighted events. Once the parton level events have been generated, a traditional parton shower (PS) Monte Carlo library can be run on top of the MADGRAPH output to describe additional QCD radiation, and possibly allow to produce hadron level generated events if a suitable hadronisation model is then applied.

In order to avoid double counting of QCD radiation from the matrix element and the parton shower, the MLM matching approach is used in its ktMLM implementation provided by the MADGRAPH team [191].

For the present study MADGRAPH-5.1.1 [191] has been used for the matrix element generation, while the parton shower and hadronisation has been provided by PyTHIA 6.4.2.4 [400]. The $W+n$ jet process has been simulated up to 4 additional partons. The PDF used in both calculations has been

CTEQ6L1, and in the matrix element calculation the strong coupling costant has been setup to be equal to the one from the PDF used. The factorisation scale and the hadronisation scale are set to the W transverse mass, $m_{\perp, W}$. The parton level clusterisation scale xqcut has been set to 10 GeV , while the ME - PS matching scale qcut has been set to the optimal value of 20 GeV , determined ensuring the smoothness of the differential jet rate.

The Pythia settings have been defined according the so called Tune Z2, an adjustment of Tune Z1 described in [450] for CTEQ6L1, where the $p_{\perp}$ cutoff for the multiple parton interactions is set to $\operatorname{PARP}(82)=1.832$ obtained on top of LHC data as far as the underlying event and multiple parton interactions are concerned, while the fragmentation parameters are those optimized on LEP data by the Professor [451] team.

Estimate of uncertainties To estimate the uncertainties due to the factorisation scale and the renormalisation scale, which are set to $m_{\perp, W}$, we varied them simultaneously by a factor two. In addition we have independently varied by a factor two the ME - PS matching scale.

While applying these modifications, the total cross-section is kept fixed to the value obtained with the default parameters, 27.77 nb . That is because we are only interested in shape variations of the distributions, rather than in the total cross-section of the process calculated by MADGRAPH, which is accurate only at the leading order.

### 18.25 PoWhEG BOX + PYTHIA8

The Powheg Box [13] is a computer framework to ease the Powheg [416] implementation of new processes. It only requires as input the individual components of the NLO calculation under consideration, i.e., the Born process, its virtual radiative corrections and the real emission contributions. Then it automatically combines them, canceling the emerging soft and collinear singularities in the Frixione-Kunszt-Signer (FKS) subtraction scheme, and produces the required events. The Powheg Box is also a library, where previously implemented processes are available in a common framework.

For the present study we make use of the $W+$ jet implementation presented in [440].
The produced events are passed to PYthia8 [348] through the Les Houches interface [452] and showered with the default transverse-momentum ordered shower, vetoing further emissions harder than the one already present in the input events. This is achieved by setting the starting scale of the shower as the transverse momentum of the hardest emission 38

When multiple partonic interactions (MPI) are turned on, these are allowed to be harder than the first Powheg emission. Indeed, since the $W+1$ jet process is not accounted for in MPI, there is no over-counting.

Eventually, the relevant distributions are evaluated by interfacing the MonteCarlo output to the RIVET [360] analysis, for the two given sets of ATLAS and CMS cuts.

Since we have simulated events starting from a hard process where a $W$ is produced in association with one jet, only observables built from events where at least 1 jet is present will be shown.

Generation of predictions and estimate of uncertainties Predictions presented here are based on a merged sample of $4 \mathrm{M} W^{+}+j$ and $4 \mathrm{M} W^{-}+j$ weighted events, produced with the default Powheg Box choice of parameters. In particular, we have required a minimum cut $p_{\mathrm{T}}=5 \mathrm{GeV}$ on the associated jet at the generation level and, in order to enhance the statistical sampling of the high- $p_{\mathrm{T}}$ tail, we have further suppressed the rapidly rising contribution at low jet $p_{\mathrm{T}}$ by the factor $p_{\mathrm{T}}^{2} /\left(p_{\mathrm{T}, \text { supp }}^{2}+p_{\mathrm{T}}^{2}\right)$, with $p_{\mathrm{T}, \text { supp }}^{2}=100 \mathrm{GeV}$. The inverse of this factor enters the event weight.

[^146]We have adopted the Powheg Box default values for EW parameters, namely

$$
\begin{equation*}
M_{W}=80.398 \mathrm{GeV}, \quad \Gamma_{\mathrm{W}}=2.141 \mathrm{GeV}, \quad\left(\mathrm{ff}_{\mathrm{em}}\right)^{-1}=128.89, \quad \sin ^{2}{ }^{`} \mathrm{~W}=0.222645 \tag{18.2.2}
\end{equation*}
$$

and we have assumed a CKM matrix with a mixing between the first two generations only

$$
\begin{equation*}
\left|V_{u d}\right|=\left|V_{c s}\right|=0.975, \quad\left|V_{u s}\right|=\left|V_{c d}\right|=0.222, \text { and }\left|V_{t b}\right|=1 . \tag{18.2.3}
\end{equation*}
$$

Finally, we have resctricted the integration region to the interval $0<M_{W}<2221 \mathrm{GeV}$.
For the computation of the Powheg $\bar{B}$ function, the renormalisation and factorisation scale was chosen equal to

$$
\begin{equation*}
\mu_{R}=\mu_{F}=p_{\perp, j} \tag{18.2.4}
\end{equation*}
$$

where $p_{\perp, j}$ corresponds to the transverse-momentum of the (single) parton recoiling against the $W$ boson in the so-called underlying Born kinematics [417]. We have also run the code using

$$
\begin{equation*}
\mu_{R}=\mu_{F}=1 / 2\left(\sqrt{M_{W}^{2}+p_{\perp, W}^{2}}+p_{\perp, j}\right) \tag{18.2.5}
\end{equation*}
$$

but no relevant differences were observed with respect to the aforementioned choice, being the two scales similar for the $W+1$ jet processes at hand.

The scales entering in the evaluation of parton distribution functions and of the strong coupling in the Powheg Sudakov form factor are chosen to be equal to the transverse momentum of the PowHEG hardest emission [417, 386].

Scale-uncertainty bands obtained by varying the factorisation and renormalisation scales entering the $\bar{B}$ function by a factor of two in either directions are used as an estimate of the theoretical error associated to higher order missing effects.

The uncertainty due to the PDF choice was estimated generating events using three different sets (CT10 [255], MSTW2008 [262], and NNPDF2.1 [312]). The value of the strong coupling constant at $M_{Z}$ is consistently read from the PDF table used. The further showering performed by PYTHIA8 is instead performed with default PDF and $\alpha_{s}$ definitions, the difference being beyond the claimed accuracy of the calculation. In this study, we have used PYthia8, version 8.153.

### 18.26 Pythias

Pythia8 [348] is the latest incarnation of event generators of the Pythia family. At the heart of the generator are parton showers that evolve high-scale processes to the scale of hadronisation, by generating splittings with DGLAP splitting kernels. The splitting scales are ordered in relative transverse momentum [348, 447], and the phase space is constructed in a dipole-like manner in order to capture soft gluon coherence effects [453]. A key point of the evolution of partonic states in PYTHIA8 is that all perturbative components are interleaved [348, 447, 454], i.e. multiple partonic interactions, space-like and time-like showers are all generated in one transverse-momentum ordered evolution sequence. This means that due to the competition for phase space, all steps in the event generation are correlated. For a detailed discussion how parameters of the interleaved shower evolution are tuned to collider data, see [455]. Pythia8 with additional matrix element corrections has so far not been tuned to data. Since in [441], only very small differences were seen for LEP between PYTHiA8 with and without matrix element merging, we expect only small re-tuning effects in the parameters of the Lund string model [456]. Similarly, since we keep the low-scale modelling of PYTHIA8 largely intact, only small changes in the underlying event tuning are expected. We however expect that some re-tuning will be needed for jet shape data.

It should be noted that Pythia8 includes a selection $2 \rightarrow 1$ and $2 \rightarrow 2$ processes, as well as a limited variety of $2 \rightarrow 3$ processes, but does not contain a general ME generator. New processes, particularly for higher jet multiplicities, have to be made available in form of Les Houches Event (LHE)
[452] files. By virtue of matrix element corrections, Pythia8 describes the first emission in $\mathrm{W}+$ jets with the full matrix element probability. When introducing matrix elements with one additional jet within matrix element merging, this allows to fully cancel the merging scale dependence for the first emission, while small merging scale dependencies enter when including further jets. Current versions of Pythia8 include a general implementation of the CKKW-L matrix element merging prescription [445]. Please consult [441] for a detailed discussion of the implementation in PYTHIA8.

Generation of the predictions To generate predictions with stand-alone Pythia8 (i.e. without inclusion of matrix elements for W production in association with two or more jets), the built-in $q \bar{q} \rightarrow \mathrm{~W}$ matrix element in Pythia8 was used to generate the initial configuration. This was then evolved with to the hadronisation scale and the ensemble of partons hadronised using the Lund string model. For this study, we use the publicly available PyTHIA 8.157, with CTEQ6L1 parton distribution functions, and the associated Tune 4C. Since [441] showed a large dependence of the quality of the matrix element merging on whether rapidity-ordered emissions are explicitly forbidden in space-like showers, results are presented with and without enforced rapidity ordering.

The inclusion of matrix elements for additional jets into PYTHIA8 is achieved with Cккw-L merging. All merging tasks are handled internally in PYthiA 8.157, allowing for a high degree of automation. This means that the user only needs to supply

- Matrix element configurations in form of LHE files.
- An identifier giving the hard process of interest.
- A value of the merging scale. Facilities to allow the user to implement a her/his own merging scale definition are available.
For this report, matrix element configurations with additional jets were generated with MADGRAPH/ MadEvent [163], and read into Pythia8 in form of Les Houches Events. Pythia8 then derives all possible parton shower histories for an event, probabilistically chooses a history, and uses the reconstructed states and splitting scales to perform a re-weighting with Sudakov factors and $\alpha_{s}$ values. This means each event will have a weight

$$
\begin{aligned}
w_{\mathrm{CKKWL}}= & \frac{x_{n}^{+} f_{n}^{+}\left(x_{n}^{+}, \rho_{n}\right)}{x_{n}^{+} f_{n}^{+}\left(x_{n}^{+}, \mu_{F}^{2}\right)} \frac{x_{n}^{-} f_{n}^{-}\left(x_{n}^{-}, \rho_{n}\right)}{x_{n}^{-} f_{n}^{-}\left(x_{n}^{-}, \mu_{F}^{2}\right)} \\
& \times \prod_{i=1}^{n}\left[\frac{\alpha_{s}\left(\rho_{i}\right)}{\alpha_{\mathrm{SME}}} \frac{x_{i-1}^{+} f_{i-1}^{+}\left(x_{i-1}^{+}, \rho_{i-1}\right)}{x_{i-1}^{+} f_{i-1}^{+}\left(x_{i-1}^{+}, \rho_{i}\right)} \frac{x_{i-1}^{-} f_{i-1}^{-}\left(x_{i-1}^{-}, \rho_{i-1}\right)}{x_{i-1}^{-} f_{i-1}^{-}\left(x_{i-1}^{-}, \rho_{i}\right)} \Pi_{S_{+i-1}}\left(\rho_{i-1}, \rho_{i}\right)\right] \Pi_{S_{n}}\left(\rho_{n}, t_{\mathrm{MS}}\right)
\end{aligned}
$$

where $\rho_{i}$ and $x_{i}^{ \pm}$are the the reconstructed shower splitting scales and momentum fractions of the incoming partons in $\pm$ z-direction, and $\Pi_{S_{+i}}\left(\rho_{i}, \rho_{i+1}\right)$ the parton shower no-emission probability when evolving the state $S_{+i}$ from scale $\rho_{i}$ to $\rho_{i+1} . \alpha_{\text {sME }}$ gives the strong coupling used in the matrix element calculation. All reweighting factors are generated dynamically with help of the shower. The interleaved evolution of PYTHIA8 is accommodated by consistently including effects of multiple interactions into the no-emission probabilities. A detailed description of the formalism is given in [441].

As input for the current analysis, we have produced LHE files for $\mathrm{W}^{+}+$jets with up to four (three) additional jets at Tevatron (LHC) energies. The renormalisation scale in MADGRaPH was fixed to $\mu_{R}=\mathrm{M}_{\mathrm{Z}}$. For hadronic cross sections, CTEQ6L1 parton distributions (as implemented in LHAPDF [457]) have been chosen at a factorisation scale $\mu_{F}=\mathrm{M}_{\mathrm{W}}$, and the strong coupling in the ME was correspondingly fixed to $\alpha_{s}\left(\mathrm{M}_{\mathrm{Z}}\right)=0.129783$. To regularise QCD divergences and act as a merging scale, a cut in

$$
k_{\perp}^{2}=\min \left\{\min \left(p_{T, i}^{2}, p_{T, j}^{2}\right), \min \left(p_{T, i}^{2}, p_{T, j}^{2}\right) \frac{\left(\Delta \eta_{i j}\right)^{2}+\left(\Delta \phi_{i j}\right)^{2}}{D^{2}}\right\} \quad \text { with } \quad D=0.4
$$

and a cut value of $k_{\perp, \min }=t_{\mathrm{MS}}=15 \mathrm{GeV}$ has been applied to the matrix element.

Merged Pythia8 predictions are given for the default settings, i.e. using the parameters of Tune 4C, for Tune A2 [458], and for Tune 4C without enforced rapidity ordering (dubbed Tune X). Again, it should be noted that so far, no tuning including additional jets has so far been conducted.

Estimate of uncertainties To estimate uncertainties of a merged prediction of W+jets, it is interesting to study the dependence on the merging scale value. For this, we have generated LHE files with three different $k_{\perp, \text { min }}=t_{\text {MS }}$ cuts $\left(t_{\text {MS }}=15,30,45\right) \mathrm{GeV}$, and performed CKKW-L merging on these samples. Furthermore, to show the effect of tuning, the $t_{\mathrm{MS}}=15-\mathrm{GeV}$-sample was processed for two adequate tunes, Tune 4C and A2.

Uncertainties related to shower ordering In [441], it was shown that restricting shower emissions in Pythia8 to regions of phase space ordered both in transverse momentum and rapidity leads to nonnegligible effects in merged predictions. This can be seen as an effect of limiting the shower accuracy by reducing the phase space over which splitting kernels are integrated, meaning the accuracy of Sudakov form factors is impaired. Loosely speaking, if above the merging scale, the matrix element, integrated over the full phase space ${ }^{39}$, differs substantially from the splitting probabilities integrated over the allowed parton shower phase space, merged results will exhibit substantial merging scale dependencies. Such problems are obviously introduced if the parton shower phase space is heavily constrained.

Changing the phase space regions in which the shower is allowed to radiate thus allows us to estimate the uncertainties of the merging procedure in conjunction with the underlying shower. Particularly, this procedure can test the quality of the matrix element merging beyond the first few emissions, and give hints on how the shower resummation may be improved.

To emphasise the impact of the shower transition probabilities, we choose a fairly small merging scale ( $t_{\mathrm{Ms}}=15 \mathrm{GeV}$ ) to regularise the tree-level matrix elements for this investigation. Then, for each matrix element state, we generate all possible parton shower histories for a matrix element state, by clustering emissions. This is achieved by inverting the shower momentum- and flavour-mappings.

When merging matrix elements with rapidity-ordered showers, we investigate two ways of biasing the selection of a particular history, from which to generate the necessary Sudakov form factors:

1. In a "y-blind" sample, we do not include an additional discriminant based on rapidity. This means that - just like in the standard case - $\rho$-ordered will be preferred over $\rho$-unordered ones.
2. In a " $y$-conscious" sample, we pick histories with rapidity-unordered splittings only if no rapidityordered histories were found. Adopting this strict ordering criterion, histories ordered in $\rho$ and rapidity will be chosen predominantly, and only if no such history exists, histories un-ordered in either $\rho$ and/or rapidity are picked.
It should be noted that to the accuracy of the parton shower, both these prescriptions are equivalent, and switching the choice of histories gives a real estimate of the quality of the merging in conjunction the underlying shower. We believe that including this uncertainty gives a pessimistic view on how wide the range of predictions of one merged calculation can be, indicating that although standard by now, matrix element merging in Pythia8 should be applied with care. However, with reasonable settings, including additional jets can improve the description of multiple hard jets substantially.

### 18.27 SHERPA

ShERPA [425, 146] is a full-fledged event generator capable of simulating all aspects of particle collisions as they occur at particle accelerators such as the Tevatron or the LHC. It includes two independent matrix element generators, AmEGIC++ [147] and Comix [459], to generate cross sections and distributions

[^147]for final state multiplicities of up to six to ten particles. In the former one, methods to automatically generate dipole subtraction terms in the widely used Catani-Seymour scheme [236, 150] have been incorporated [448]; the SHERPA package also supports the BLHA [145] for the interface to one-loop programs such as BlackHat or GoSam. For parton showering, SHERPA employs an algorithm based on Catani-Seymour subtraction kernels, proposed in [460] and implemented in the SHERPA framework in [461]. For the hadronisation, SHERPA uses either its native hadronisation scheme, based on the cluster fragmentation model [462] and its implementation described in [463] or an interface to PYtHIA [400] providing access to the routines of the Lund string model [456]. Both have been successfully tuned to LEP data within the SHERPA framework, with a similar quality in describing the data. The hadron decays are also fully provided in the SHERPA framework, as well as QED final state radiation to both the $W$-boson and the hadron decays, simulated using the YFS approach [464, 465].

In this work, the most recent, publically available SHERPA version, SHERPA-1.3.1, has been used in two ways of running the simulation, namely

1. in the MEPs mode:

In this method, towers of LO matrix elements with increasing jet multiplicity, in the case at hand $W, W+1, W+2, \ldots, W+n_{J}$ jets, are merged in the spirit of [429, 430] to yield an inclusive sample. In fact, codes relying on such algorithms have been compared in a previous publication [439], which helped to establish and validate the methods and their various implementations. In contrast to the original implementation in SHERPA [466], which used analytical forms of Sudakov form factors etc., the current version of the method [426] directly uses the parton shower for Sudakov rejections etc. and is thus closer in spirit to the variant presented in [445, 467] for multijet merging.
2. in the MENLOPs mode:

This method can be understood as the combination of a matching of the parton shower to a NLO matrix element and a merging of additional towers of LO matrix elements with even higher jet multiplicities. Thus, in the case at hand, inclusive $W$ production calculated at NLO accuracy is merged, as above, with LO matrix elements for $W+1, W+2, \ldots, W+n_{J}$ jets. This method has been pioneered in [442, 443] where the implementation employed within Sherpa has been detailed in the second reference.

The respective settings and relevant details for both simulation modes are described below.

Sherpa in MePs mode In the MEPS mode Sherpa was run with up to $n_{J}=6$ jets in the matrix element evaluation including all possible massless (anti-)quark and gluon initial and final states. All matrix elements were generated using Comix. The MEPS-separation parameter was set to $Q_{\text {cut }}=20 \mathrm{GeV}$, for its precise definition see [426]. The scales are chosen as

$$
\begin{equation*}
\alpha_{s}^{k+n}\left(\mu_{\mathrm{eff}}\right)=\alpha_{s}^{k}(\mu) \cdot \alpha_{s}\left(p_{\perp, 1}\right) \cdot \ldots \cdot \alpha_{s}\left(p_{\perp, n}\right), \tag{18.2.6}
\end{equation*}
$$

wherein the relative transverse momenta $p_{\perp, i}$ are the nodal values of the final state partons of the $W+n$ parton matrix element as obtained from recombining it using the inverted splitting probablities given by the parton shower. The core scale $\mu$ is then chosen as the partonic centre-of-mass energy of the reconstructed core process, i.e. $\mu^{2}=\hat{s}_{2 \rightarrow 2}$ where $k=0$ in the process at hand. In all stricly perturbative setups a parton shower cutoff of $t_{0}=(0.7 \mathrm{GeV})^{2}$ has been used.

The parton shower cutoff and all fragmentation parameters of both the internal cluster hadronisation and the interfaced Lund string fragmentation models have been tuned to LEP data and give a similarly good description. Similarly, the parameters of SHERPA's MPI model have been tuned to Tevatron and LHC data using the CT10 [255] parton density parametrisation. These parameters are given in App. 18.71

Sherpa in Menlops mode In the MeNloPs mode Sherpa is run with essentially the same parameters as in the MEPs mode, described in the previous subsection. Hence, $n_{J}=6$ and $Q_{\text {cut }}=20 \mathrm{GeV}$. To be able to describe the inclusive $W$ production process at NLO accuracy, AmEGIC++ was used for all parts of the NLO $W$ production matrix elements (supplemented with a hardcoded one-loop matrix element from the internal library) and the LO $W+1$ parton matrix element. Consecutively, the scales were chosen as above with $k=0$ for all tree-level parts and $k=1$ for the real and virtual corrections entering the next-to-leading order correction of the core process. All non-perturbative parameters remain unchanged wrt. the MEPS mode.

Estimate of uncertainties In order to estimate the uncertainites of the SHERPA predictions, the following procedures have been applied:
(A) PDF uncertainties:

Unlike in the PDF4LHC presciption [468], here only the central predictions of the three NLO PDFs, CT10 [255], MSTW2008 [262] and NNPDF2.1 [312] are compared to estimate the PDF uncertainties. The different parametrisations of PDFs as well as their corresponding value of $\alpha_{s}$, both its value at $M_{Z}$ and its running, enter in the calculation of the matrix elements, the parton shower and the underlying event.
(B) Scale uncertainties:

In a global manner, all scales, renormalisation and factorisation scales are simultaneously modified by the canonical multiplication with 2 and $1 / 2$. This, however, is not only applied to the evaluation of the matrix elements but also to that of the parton shower, the hadronisation, the underlying event simulation and the hadron decays. Regarding the matrix-element evaluation, the MEPs default scale choice forms the starting point for the scale variations to be executed.
(C) Hadronisation uncertainty:

Here the intrinsic modeling uncertainties are evaluated by changing the hadronisation model operating on SHERPA's parton shower final states, namely switching from SHERPA's default cluster hadronisation to PYTHIA's string fragmentation. For both schemes, an independently tuned set of parameters has been employed to perform the parton-to-hadron transition.
(D) Underlying event uncertainty:

To this end the tune of the underlying event based on using the CT10 PDF has been modified such that the plateau of the number of charged particles and sum of transverse momenta in the transverse region are increased or decreased by $10 \%$. This change in the amount of MPI activity is accomplished by varying the $\sigma_{\mathrm{ND}}$ correction factor (SIGMA_ND_FACTOR) by -0.04 or +0.05 , respectively.

### 18.3 Results

In this section we compile results for the individual codes for a number of representative observables at the different levels of the simulation. It should be noted, though, that in all results presented in this section PDF uncertainties have been estimated by typically varying only over a few different sets rather than employing the full procedure as suggested by the PDF4LHC accord [468].

### 18.31 BLACKHAT + SHERPA

The following results have been obtained with BlackHat+SherPa. Uncertainties due to the factorisation/renormalisation scale variation and the that due to the PDF uncertainties are shown. The yellow band corresponds to the addition in quardature of these two uncertainties and the statistical estimation on the integration error. All observables are defined using the ATLAS cuts, cf. App. 18.6.

Fig. 64 displays the inclusive cross section for a $W$ boson in association with $n$ jets, where $n=1,2,3,4$. A NLO computation of $W+4$ jets also provides a leading order calculation of the $W+5$
jets rate, but since it is not at NLO accuracy we refrain here from including it.
In all the plots presented in this section the uncertainties are dominated by the uncertainty arising from the scale variation (it is not the case when the central scale of the process is chosen close to a local maximum, in which case the upper boundary of the scale variation is very close or identical with the central value, as can be seen from the plots corresponding to $W+3,4$ jets). This is partially due to the fact that for the assessment of the PDF uncertainty only error sets have been employed that are closely related to the central set. In addition, the functional form of the scale definition as given by the kineamtics of the final state has not been changed, but rather the emerging scales $\mu_{F}$ and $\mu_{R}$ have been multiplied in parallel by factors of 2 and $1 / 2$.


Fig. 61: Pseudo-rapidity and transverse momentum distributions for the first jet in inclusive $W+1$ jet production (upper panel), for the second jet in inclusive $W+2$ jet production (central panel), anf for the third jet in inclusive $W+3$ jet production (lower panel).


Fig. 62: Pseudo-rapidity and transverse momentum distributions for the fourth jet in $W+4$ jet production.


Fig. 63: HT distributions for event with at least one (top left), two (top right), three (bottom left) or four (bottom right) jets.


Fig. 64: Inclusive cross section for $W+n$ jet production.

### 18.32 GoSAM + SHERPA

The setup described in the previous section for the analysis using GoSAM+SHERPA gives the following theoretical uncertainties. The plots show that in general the scale uncertainties are bigger then the PDF uncertainties and that the renormalisation scale dependence is usually bigger then the dependence on the factorisation scale. To illustrate the decrease in the scale uncertainty given by the NLO calculation we also include the distributions for the pseudo-rapidity and transverse momentum of the second hardest jet, which have only tree-level accuracy. All observables shown are defined using the ATLAS cuts, cf. App. 18.6 Note that errors in the 2 -jet configuration are increased w.r.t. those provided by BLACKHAT+SHERPA, since here only $W+1$ jet configurations are dealt with at NLO, and the 2 -jet configurations therefore are descibed at LO only.


Fig. 65: Pseudo-rapidity and transverse momentum distributions for the hardest jet.


Fig. 66: Pseudo-rapidity and transverse momentum distributions for the second hardest jet. This distribution have formally leading order accuracy and have therefore a much larger scale dependence than the same distribution for the hardest jet, for which a genuine NLO prediction is available.


Fig. 67: HT distributions (left) and $\Delta R$ between lepton and hardest jet (right) for events with at least one jet.

### 18.33 HEJ

This section contains the predictions from the High Energy Jets (HEJ) event generator. This gives predictions for the production of a $W$ boson in association with at least two jets. Throughout, we show results for CTEQ, MSTW and NNPDF parton distributions. We show a scale uncertainty band only for the first of these for clarity. The results for the other two are very similar. The yellow band in the ratio panel shows the statistical uncertainty in each case. The scale variation is seen to be dominant over the statistical uncertainty and the differences in choice of pdf. All observables are defined using the CMS cut definitions, cf. App. 18.6

As discussed in Sec. 18.23, the resummation contained in the HeJ framework is supplemented with a merging procedure to ensure tree-level accuracy for events with up to and including four jets. This leads to the larger drop from the four jet to the five jet cross section, compared to the drop either from


Fig. 68: The Hes prediction for the distribution of the transverse mass of the $W$ boson (top left) and for the angle between the hardest jet and the charged lepton from the decay of the $W$ boson (top right), the transverse momentum of the hardest jet (bottom left) and for the $H_{T}$ distribution (bottom right) in events where a $W$ boson was produced in association with at least two jets.


Fig. 69: The Hes prediction for the cross sections of $W$ plus $n$ jets.
three-jet to four-jet, or from five-jet to six-jet. This can be clearly seen in Fig. 69

### 18.34 MadGraph + PYthia

The following results have been obtained with MadGraph+Pythia. Uncertainties due to the factorisation and renormalisation scale and MEPs matching scale are shown for results on hadron level including UE and QED final state radiation. A comparison of results on parton shower level, hadron level, hadron level including UE, and hadron level including UE and QED final state radiation, is also presented. All observables shown are defined using the CMS cuts, cf. App. 18.6.

From these results we can conclude that the largest uncertainty on all observables is due to the factorisation and renormalisation scale. In addition to that, a large effect is found by switching off the final state QED radiation, while only a small difference is oberved between results at the shower level and all other results prior to the QED radiation.


Fig. 70: MadGraph + Pythia results for $W$ transverse mass.


Fig. 71: MADGraph+PYTHIA results for $\Delta R$ between lepton and hardest jet.


Fig. 72: MadGraph+Pythia results for for $p_{\perp}$ of hardest jet (top), number of jets (middle) and $H_{T}$ of events with at least 2 jets (bottom).

### 18.35 Powheg Box + Pythia8

In this section we show results obtained by running the Powheg Box implementation of $W+1$ jet together with Pythia8. In all the following plots of this section, CMS analysis cuts have been enforced, see App. 18.6. For this study, in the left panels of Figs. 73.75, we show uncertainties obtained from variations of renormalisation and factorisation scales by a factor of two in either directions and by choosing different PDF sets in the computation of the hard scattering. Results are shown at the final level, after the shower, the hadronisation and the inclusion of MPI, all performed by PYTHIA8. In general, we notice that the uncertainty due to scale variations is greater than the changes in the results due to different PDF choices.

In the right panels of Figs. $73 / 75$ we show our results at different stages of the simulation, for a fixed PDF set (chosen to be CT10). The stages considered include from the first emission level up to the full showered events in PYTHIA8, including MPI and also effects due to QED radiation off leptons and quarks. Various stages of the simulation have been obtained setting the PYTHIA8 switches as reported in Sec. 18.73 .

We recall here that results should be considered to be physical only after the the hadron level is reached (possibly including MPI and QED effects). In particular, we stress that the results at the parton level are obtained considering only the POWHEG first emission, and they are therefore only intermediate: indeed at this stage only the hardest radiation has been generated and effects due to further showering are not yet taken into account.

For most of the observables results do not show large variations going from a simulation level to another. In particular, for truly NLO predictions such the plots in Fig. 74 or the bin $n_{\text {jet }}=1$ of Fig. 73 , the major effects that arise at each successive stage of the simulation are a change in the normalisation, due to a slightly different number of events passing the analysis cuts when multiple emissions are allowed, and a moderate shape distortion in the low end of the spectrum. Both these effects may be attributed to multiple QCD radiation due to Sudakov effects introduced by the parton shower. As expected, these effects are of the same size, or smaller, than the theoretical uncertainty due to scale and PDF's variations, when propagated to the hadronic level. Similar effects are also observed when the QED radiation is turned on. In this case, results are lowered as a consequence of the cuts on the lepton transverse momentum and rapidity.

Due to the requirement of having at least two jets, the remaining observables are predicted only at leading order or with leading log accuracy by the Powheg simulation of $W+1$ jet. This is also reflected


Fig. 73: The number of jets, as predicted by Powheg Box + Pythia 8 .


Fig. 74: The hardest jet transverse momentum distribution (upper plots), the $\Delta R$ separation (middle plots) and the invariant mass $m$ (lower plots) of the hardest jets and the hardest lepton, as predicted by Powheg Box + Pythia8.


Fig. 75: The transverse momentum $p_{\perp}$ of the next-to-hardest jet, the scalar sum of the jet transverse energy $H_{T}$ of events with at least 2 jets and the sum of the transverse energies of all the particles in events with 2 or more jets, as predicted by Powheg Box + Pythia8.


Fig. 76: Comparison between predictions using different PYTHIA8 tunes, at hadron level with MPI, as predicted by Powheg Box + Pythia8.
in the larger band associated with the scale variations.
Observables such as $H_{T}$, the scalar sum of the transverse energy of the jets for events with two or more jets, show an enhancement in the high- $H_{T}$ tail. This effect mostly arise as a consequence of the showering, since the successive stages do not change the predictions any longer. The same behaviour, even more enhanced, is also observed in the scalar sum of the transverse energy of all particles, always in events with two or more jets.

In Fig. 76 we instead compare the effect of using different PYTHiA8 tunes on our predictions, obtained in this case at the hadron level, including MPI. Essentially all the observables turned out to be extremely stable under the variations of the PYthia8 tune, as shown in Fig. 76. Major differences only appears for the beam thrust, when it is defined at the particle level (see App. 18.62).

### 18.36 Pythias

For this study, PYthia8 has been run stand-alone and including matrix elements with additional jets. Note that in PYthia8, multiple interactions are interleaved with space- and time-like showers, meaning that in general, MPI and parton showers cannot be disentangled by just switching off secondary scatterings. When referring to "Hadron Level", we mean after the interleaved evolution (including QED


Fig. 77: Tuning variations for Pythia8 at hadron level. The plots show the $H_{T}$-distribution when requiring at least two jets (upper left), the $p_{\perp}$ of the hardest jet (upper right), the $\Delta R$-separation of lepton and the hardest jet (lower left), and the number of jets (lower right). The lower insets show the ratio of the samples in the upper half to ME3PS (Tune 4C, y-blind treatment). All merged plots are produced with a merging scale of $t_{\mathrm{MS}}=15 \mathrm{GeV}$.
splittings), and after hadronisation. For the sake of comparison, "Shower Level" indicates results after (interleaved) final- and initial-state radiation, switching multiparton interactions off. All results presented in this section are generated with CTEQ6L1 parton distributions for protons colliding at $E_{\mathrm{CM}}=7000$ GeV . Cккw-L-merged samples include up to three additional jets, taken from MADGraph/MadEvent.

Fig. 77 exemplifies how changes in the tuning of the event generator can affect the outcome of merged calculations in PYTHIA8. For this, we produce predictions for Tune 4C [455] and Tune A2 [458]. In general we observe only modest shape changes of up to about $20 \%$ in observables, when comparing the two merged predictions, lending confidence to the statement that the tuning did not artificially produce hard scale physics. Normalisation changes between 4 C and A2 can be explained by a difference in Sudakov suppression: Since Tune 4C integrates the splitting kernels over a smaller region of phase space, the suppression generated by trial showers is less pronounced. The increase in the number of jets in Tune A2 with respect to Tune 4C, after the third jet, is expected, because the generation of the fourth jet is handled solely by the parton shower. Since 4C allows less phase space for these emissions by


Fig. 78: Variation of the merging scale value for Pythia8 at shower level. The plots show the $H_{T^{-}}$ distribution when requiring at least two jets (upper left), the $p_{\perp}$ of the hardest jet (upper right), the $\Delta R$-separation of lepton and the hardest jet (lower left), and the number of jets (lower right). The lower insets show the ratio of the samples in the upper half to ME3PS for $t_{\text {MS }}=30 \mathrm{GeV}$. All plots are generated using Tune 4C (y-blind treatment).
enforcing rapidity ordering, A2 will look harder. It is debatable whether including rapidity ordering into the tuning makes the tune mimic hard scale effects. The scales at which the fourth jet is produced are certainly close to the scale of (hard) multiple interactions, which is in turn closely connect to soft physics. Although the enforced rapidity ordering in Tune 4C might be considered questionable, we here take the pragmatic approach of considering the evolution both with and without enforced rapidity ordering. From the fact that up to three jets, the merged predictions of Tune 4C and Tune A2 only differ in normalisation, we anticipate that the effect of rapidity ordering will be reduced by merging more jets, since then, the number of jets above a cut-off will be dictated by the matrix element.

In Fig. 78, we investigate the impact of changes in the merging scale value. Again, we mainly see normalisation changes and only small changes in shape, which in most cases are smaller than changes due to different tunes. The $R$-separation between lepton and hardest jet $\Delta R$ (lepton, hardest jet) shows significant shape changes above $\pi$. This again is an effect of Tune 4C, and is greatly reduced in Tune A2 $2^{40}$, as

[^148]

Fig. 79: Variation of the criterion employed to favour "ordered histories" in Pythia8 at shower level. The plots show the $H_{T}$-distribution when requiring at least two jets (upper left), the $p_{\perp}$ of the hardest jet (upper right), the $\Delta R$-separation of lepton and the hardest jet (lower left), and the number of jets (lower right). The lower insets show the ratio of the samples in the upper half to ME3PS (Tune 4C, y-blind treatment). All merged plots are produced with a merging scale of $t_{\mathrm{MS}}=15 \mathrm{GeV}$.
can be inferred from the tune variation. However, even in Tune A2, small shape changes remain, with the change becoming less pronounced when comparing two large merging scales. We take this as an indication that the shower splitting probability - giving radiative contributions to $\Delta R$ (lepton, hardest jet) $>\pi$ for high $t_{\mathrm{Ms}}$ - and the the matrix element, which fills the same region in for the low merging scale case, are indeed different from the second jet on. This also explains the difference between Tune 4C and Tune A2, which differ by the phase space regions over which the splitting kernels are integrated.

Finally, in Fig.79, we address the interplay of matrix element merging and ordering in the underlying shower more carefully. The effect of different choices manifests itself again mainly in changes of the normalisation of the plots, and is comparable in magnitude to the impact of merging scale variations. At first, the changes may seem counter-intuitive, and need clarification. For this, it is important to remember the definition of " y -blind" and " y -conscious" in section 18.26 . The y -blind treatment will - irrespectively of rapidity configurations - mainly choose histories ordered in the shower evolution variable $\rho$, and only

[^149]pick $\rho$-unordered histories if no other ones have been constructed. However, in the y-conscious approach, once no history ordered both in rapidity and $\rho$ is found, one amongst all un-ordered histories is chosen probabilistically, irrespectively of the history being y-/ $\rho$-/or y- and $\rho$-unordered. Since the ordering criterion is stricter, un-ordered histories will be chosen more frequently, meaning that $\rho$-unordered ones will also contribute more, compared to the y-blind case. Matrix element states with no ordered histories will have a number of jets at very similar scales, so that the Sudakov suppression generated by trial showers will be smaller. Moreover, for matrix element states in which the last reconstructed splitting is unordered, the parton shower will be started at the larger of the unordered scales ${ }^{41}$, which can result in a slightly harder spectrum of resolved parton shower jets. Because $\rho$-unordered states are picked more often when requiring a tighter ordering criterion, this leads in visible differences. The y-conscious method might seem somewhat artificial, considering that it introduces a larger dependence on states outside the range of even the $y$-unordered shower variant. Nevertheless, the $y$-blind and $y$-conscious prescriptions are equivalent to the accuracy of the (y-ordered) shower, so that both should be investigated when assessing the quality of the merging. From the visible changes, we can infer that different treatments of formally sub-leading effects do matter. For the y-ordered evolution, these are more visible since the accuracy of the shower itself is worse, so that the effects of including matrix element states cancel to a lesser degree. It is interesting to note that the deviations between the different prescriptions are considerably smaller if the merging scale is increased, again hinting at a reduced shower accuracy if the evolution is ordered in multiple variables.

Fig. 79 further shows distributions labelled Tune $X$, which have been generated by using Tune 4 C , removing the rapidity constraint on space-like emissions, and treating histories y-blind. Results of these runs, as expected, closely follow Tune A2. The outcome of both Tune A2 and Tune X differs only slightly from the Tune 4 C (y-blind) curves, consolidating the conclusion that shifting fractions of $\rho$-un-ordered histories are responsible for the deviations between the y-blind and y-conscious methods. As in the discussion of tuning variation, the similarity in the results of the merged calculation for Tune 4C and Tune A2 breaks down once we examine jets that are solely produced by the shower, i.e. starting from the fourth jet.

### 18.37 SHERPA

As described in Sec. 18.27 , SHERPA has been run in two modes for this comparison of LHC predictions. The results for the conventional merging of towers of tree-level matrix elements, SHERPA MEPS, are presented in Sec. 18.37 while the results of its enhancement to NLO accuracy in the core $W$ production process, Sherpa MeNloPs, are displayed in Sec. 18.37 . As detailed earlier, all parameters have been chosen identically otherwise. The precise requirements regarding the event selection and the definitions of the observables used in this comparsion follow the CMS cut specifications and can be found in App. 18.6.

SHERPA MEPS Figs. 80,83 show the results as obtained by running SHERPA in the MEPS mode for a variety of inclusive and multi-jet observables at different levels of the event generation. All central results are displayed together with their respective uncertainties related to the different sources listed in Sec. 18.27. The layout in all figures is the same: the upper left and right panels respectively show the matrix element level and parton shower level predictions for a given observable. The matrix element level is defined as the event generation phase right before the parton showering. For the MEPs approach this means that modifications necessary for the procedure to work like $\alpha_{s}$ reweighting and Sudakov rejection have been already included at this level. The predictions presented in all centre panels were generated after enhancing the event generation to include corrections induced by the parton-to-hadron transition and decays of the therein produced primordial hadrons. On top of these soft physics effects, one has to also

[^150]

Fig. 80: SHERPA MEPS. Uncertainty of the transverse mass of the reconstructed $W$ on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 81: Sherpa MePs. Uncertainty of the angular separation of the charged lepton and the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 82: SHERPA MEPS. Uncertainty of the transverse momentum of the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 83: Sherpa MEPs. Uncertainty of the inclusive jet multiplicity on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.
account for multiple parton interactions. The results in the centre right panels of all figures incorporate these additional corrections. Finally, all plots to the lower left show the most complete hadron level predictions, which were obtained by adding to the event generation QED radiation effects as occurring in the decays of the vector boson and the hadrons. To allow a direct comparison of the impact of the consecutive event stages, the way the central results change is summarized in all plots to the lower right of Figs. 80.83 . In these, as in all other panels, the main plots are supplemented by ratio plots stressing the magnitude of the differences and uncertainties. Note that the yellow band throughout illustrates the statistical uncertainty on the central event sample.

Apart from the summary plots at the lower right, all other cases depict predictions documenting the uncertainty of the central predictions at the different levels of event generation. These uncertainty estimates are gained following the procedures outlined in Sec. 18.27. At all event simulation phases, the scales are varied as described under this section's point (B). Note that the variation is applied to all phases used to make up the respective central (or default) sample, which is taken as the reference under all circumstances. For the matrix element level, parton shower level and full hadron level results, PDF variations according to point (A) are shown in addition, whereas for the centre panel plots, the focus is on the outcomes of the model and tune variations instead, as specified in point (C) and point (D) of Sec. 18.27. Notice that the lower left panels also contain the outcomes of scale variations utilizing the alternative PDFs mentioned under point (A); they are much alike the ones stemming from the default set.

As an example for an inclusive observable the transverse mass of the reconstructed $W$ boson is shown in Fig. 80. The scale uncertainties amount to $\sim 15 \%$ at all generation levels, whereas the uncertainties due to the choice of PDF are much smaller. Similarly, the hadronisation uncertainty is negligible. The $m_{\perp, W}$ observable however is more sensitive to the tuning of the MPI model as can be seen from the $\pm 10 \%$ envelope in the centre right plot of Fig. 80. The uncertainty is of the same order as for the scale variations, which generally are more pronounced in the soft region. When considering the impact of each perturbative and non-perturbative event stage (see the plot to the lower right), it is the MPI corrections that are largest in the region of $m_{\perp, W}<m_{W}$, ranging up to $\sim 30 \%$ wrt. the matrix element level prediction. They are small above $m_{W}$. In this region the dominant effect comes from the QED corrections, which themselves are rather small, but they lead to a contamination of the electron isolation. The application of the isolation cuts then yields a reduction of the overall normalisation of the event sample. Finally there is a small shift towards lower transverse masses, pronouncing the deviation in the tail of the distribution somewhat further.

Fig. 81 and Fig. 82 depict observables that require the presence of at least one jet. In the former the geometric separation, $\Delta R$, between the hardest jet and the electron is shown, while in the latter, focus is on the transverse momentum, $p_{\perp}$ of the hardest jet only. As before the dependence of the predictions on PDF and hadronisation model changes remains negligible. While the scale dependence of the $\Delta R$ and $p_{\perp}$ variables increases to $\sim 30 \%$, the uncertainty due to the tuning of the MPI model decreases to $\sim 5 \%$ when compared to the findings concerning the more inclusive observable considered above. In both cases the reason for the sensitivity change obviously lies in demanding at least one (hard) jet. The scale uncertainties primarily result from changes in the overall cross section. Again, comparing the results of the different event stages, one clearly observes the large impact parton showering has on modifying the matrix element level predictions. The non-perturbative effects go in the same direction amplifying the parton shower effects, but as expected this amplification turns out to be rather mild in the well separated and/or hard phase space regions. QED corrections only play a minor role, and are far less important than for the $m_{\perp, W}$ variable.

In Fig. 83 one of the simplest examples of a multi-jet observable is presented, namely the distribution of the inclusive $W+n$ jet cross sections as a function of $n_{\text {jet }}$. Qualitatively, the parameter and model dependencies of the predictions are found to behave as for the inclusive one-jet variables. As one would expect, the scale uncertainties subsequently increase with the order of the jet bin. The same can be noticed for the variation of the PDFs used in the calculation - even though here the effect is considerably
smaller.

Sherpa MeNloPs Following the outline of the previous subsection, Figs. 84.87 compile the results, which were obtained by executing SherPa in the MENLoPs mode, cf. Sec. 18.27. The presentation is based on the same set of figures where the selection of the observables has been taken as in the MEPS case. Again, all (central) predictions are examined towards their scale, PDF, non-perturbative modeling and QED simulation dependence. One small difference has to be pointed out: the plots to the lower left now depict exclusively to what extent the additional QED corrections modify the outcomes including multiple parton interactions and hadronisation effects.

Fig. 84 shows the transverse mass of the reconstructed $W$ boson. In the MENLOPs approach, this observable is described at NLO accuracy, which leads to a reduction of the associated scale uncertainties. The scale variation results for $m_{\perp, W}$ nicely confirm this expectation as can be seen in the upper four plots of Fig. 84. The deviations from the central prediction are much smaller than those found for the MEPs scenario exhibited in Fig. 80, they now are of similar magnitude as the PDF uncertainties. While the scale dependence is reduced, PDF and MPI tune variations as well as QED corrections manifest themselves as in the MEPS case. In particular, the discussion around Fig. 80 explaining the effects of extra QED emissions (as being most relevant in the $W$ decay) can be used to understand the findings illustrated in the bottom left panel of Fig. 84

The MENLOPs method primarily improves the precision of the description of the core process, here the description of the $W$ production process. One also benefits from improving the overall normalisation. However, processes with additional partons in the final state are described in the MENLoPs approach at the same level of accuracy as in the MEPS approach - in both cases by tree-level matrix elements. Thus, the one-jet observables, $\Delta R$ between the lepton and leading jet and the $p_{\perp}$ of the leading jet, and their related uncertainties turn out to be predicted in a very similar manner. This can be clearly observed by comparing Figs. 85486 with Figs. $81 / 82$. Unlike the findings for $m_{\perp, W}$, it particularly can be noticed that the scale dependence associated with the one-jet observables shown here remains unchanged when compared to the respective MEPS results.

Fig. 87 depicts the distribution of the inclusive $W+n$ jet cross sections as obtained for the MeNloPs case. Using the above reasoning, one can understand these results as for the one-jet variables. Note that the scale dependence of the zeroth jet bin shows the expected decrease owing to the NLO accuracy underlying the description of the core process.

Fig. 88 finally, highlights the evolution and uncertainties of two definition of the beamthrust, cf. App. 18.6 a physical observable summing over all final state particles excluding the $W$-constituent lepton and a pseudo-observable including the $W$ itself. For both observables small perturbative uncertainties are completely burried underneath much larger non-perturbative effects and modelling uncertainties, an effect also seen in results from the Powheg Box+Pythia simulation, cf. Fig. 76. This can only be interpreted as this observable being dominated by non-perturbative effects and in particular the underlying event, which somewhat invalidates statements about the merit of this observable in a clean determination of initial state radiation effects made in [469, 26].


Fig. 84: Sherpa MeNloPs. Uncertainty of the transverse mass of the reconstructed $W$ on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 85: Sherpa MeNloPs. Uncertainty of the angular separation of the charged lepton and the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 86: Sherpa MeNloPs. Uncertainty of the transverse momentum of the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 87: Sherpa MENLoPs. Uncertainty of the inclusive jet multiplicity on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 88: Sherpa MeNloPs. Evolution and uncertainty of two definitions of the beamthrust, calculated using all particles not constituting the $W$ (left) and including the $W$ (right). Exemplary, the combined PDF and scale uncertainty on the matrix element level prediction (yellow) and the modeling uncertainty of the hadron level prediction (blue) are shown.

### 18.4 Comparisons

In this section we compare the results of different tools with each other. While the aim of this study was to have a fairly tuned comparison with as many aspects of the calculations as possible being centrally defined, there are still important residual differences in the various results. Obviously, the different codes produced results at different stages of the simulation, which are not always directly comparable; in addition, some of these stages are not very straightforward to obtain: for instance, running PyTHIA8 without multiple parton interactions included in the interleaved showering obviously changes the overall logic of the parton shower model of this code. In addition, other, more obvious differences occur, ranging from inconsistent choices of PDFs to different strategies in scale setting procedures. For the case of the PDFs, by directly comparing results obtained with BlackHat+SHERPA using CTEQ6.6 and with GoSAM+SHERPA using CT10, it appears as if at NLO these differences are minor. However, it is not clear how much of the differences between MADGraph+PYTHIA and PYTHIA8, which both employ CTEQ6L1, and the other codes, which employ NLO PDFs, can be attributed to differences in PDFs.

In addition, results obtained with the NLO codes typically include at least one jet - Powheg Box+Pythia8 and GoSam+Sherpa take $W+1$ jet at NLO as their core process - while Hej starts at $W+2$ jets, and BlackHat+Sherpa presents results for up to 4 jets accompanying the $W$ boson in different jet bins. Obviously, on the other hand, the multijet merged samples of MadGraph + PYthia, Pythia8 MePs and Sherpa include LO matrix elements for up to 3 to 6 jets.

In the plots in this section each code is shown with a yellow error band, which is the envelope of the variations presented in Sec. 18.3. The only exception is BLACKHAT+SHERPA, which is shown with a blue error band. In the ratio plots the codes are plotted relative to BLACKHAT+SHERPA, also at the parton shower level.

### 18.41 Inclusive observables

In this section we present some inclusive observables, which are typically all obtained from codes employing multijet merging. By and large, all codes agree in the shapes of the $m_{\perp, W}$ distribution at different stages, although there are sizable differences in the respective normalisation of the samples.


Fig. 89: Transverse mass of the reconstructed $W$ on all levels of the simulation, for the exact definition see App. 18.62 and for the cuts employed in the analysis App. 18.61 Note that PyTHIA8 and MadGraph+PyTHia use the CTEQ6L1 pdf, while Sherpa uses CT10.

### 18.42 Observables with at least one jet

As a first and fairly telling observable the $p_{\perp}$-spectrum of the hardest jet is compared, cf. Fig. 90, At the parton level, the results of the NLO calculations - BLACKHAT+SHERPA and GOSAM+SHERPA- agree nearly perfectly with each other and within about $20 \%$ with the multijet merged samples of SHERPA, both at LO (Sherpa MePs) and in the MeNloPs (Sherpa MenloPs) sample. The increase of the latter with respect to the former at relatively low transverse momenta of about 50 GeV or below can probably be related to the different scale definition in the argument of the strong coupling, where the NLO calculations choose $\mu_{R}^{2}=\left(H_{T}^{\prime} / 2\right)^{2} \approx M_{W}^{2} / 4+p_{\perp, j}^{2}$ while in the SHERPA simulation the transverse momentum of the jet has been chosen. Clearly, for small transverse momenta this will lead to visible differences. Going from the matrix element to the parton shower level typically leads to the jets becoming softer and to losing some of them, due to partons emitted outside the jet and a corresponding energy loss. This explains why the SHERPA distribution at the shower level is softer than the NLO result, and thus the SHERPA result at the matrix element level, although the size of the difference seems to be larger than one would naïvely expect. This finding is, however, somewhat at odds with the results obtained from MADGRAPH+PYTHIA, which seem to be slightly harder in shape and significantly larger in normalisation. The PYthia8 MEPS sample, on the other hand, has a smaller one-jet inclusive cross section than SHERPA, but the jet spectrum exhibits a somewhat harder tail, corresponding to a shape difference of about 30$40 \%$ with respect to both the Sherpa results. The same finding, a somewhat harder tail, is also true for the Powheg Box+Pythia8 results. The same trends can be also found at the hadron and hadron + MPI level. For the Powheg Box result the difference can be attributed to the usage of a scale defined at the "underlying-Born" level (cf. Sec. 18.25 for more details). Indeed it has been checked explicitly that a NLO computation performed with the same scale choice used in Powheg Box gives a result in complete agreement with the POWHEG Box result shown here. Clearly, the differences between different


Fig. 90: Transverse momentum of hardest jet on all levels of the simulation, where jets are reconstructed using the anti- $k_{\perp}$ with $R=0.4$ within $|\eta|<4.4$ (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BlackHat+ShERPA (on matrix element level).
calculations and codes exhibited here deserve a more in-depth study, which, unfortunately, is beyond the scope of this comparison.

Similar findings are also true for the next observable, the $\Delta R$ distribution between the lepton stemming from the $W$ decay and the hardest jet displayed in Fig. 91. Again, the two Sherpa samples are compared with the two NLO samples, this time exhibiting a sizable shape difference towards an increase at smaller and a decrease at larger distances of about $40 \%$ relative cross section. While higher jet configurations typically tend to be a bit more central, it seems far-fetched to attribute this difference only to them. At the same time, large differences in $R$ are most likely due to jets which are pretty much forward ${ }^{42}$. This region of phase space for jet production, however, is known to be quite susceptible to mismatches in scale and/or PDF definitions. However, it is worth noting that this difference vanishes almost completely at the parton shower level. The Pythia8 MEPs sample, despite a sizable difference in cross section, appears to follow the shape of the NLO and SHERPA results. Further comparing these results to those of the other codes at the shower level suggests that the MadGraph+Pythia merged sample, apart from a drastically enhanced cross section, also shows an enhancement in shape at smaller $\Delta R \leq 2$ w.r.t. the NLO result. Interestingly enough, the Powheg Box+Pythia8 sample exhibits the

[^151]

Fig. 91: $\Delta R$ between hardest lepton and hardest jet on all levels of the simulation (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).
opposite behaviour: while the cross section seems fairly consistent with the SHERPA and the NLO ones, the shape shows some enhancement of up to $40 \%$ at large distance $\Delta R$, which following the reasoning for the jet $-p_{\perp}$ spectrum may also hint at being due to a difference in the definition of scales. As before, the same trends visible at the parton shower level can also be found at the hadron and hadron + MPI level.

### 18.43 Multi-jet observables

In observables including at least two jets, consider first the case of the $H_{T}$ distribution depicted in Fig. 92 , Over the full range and obscured by large statistical fluctuations both SHERPA samples seem to follow the NLO prediction from BlackHat+Sherpa. The LO result from GoSam+Sherpa, on the other hand, appears to fall off at the hard end of the distribution. The prediction from HEJ is a bit more subtle to judge: at low $H_{T}$ (around 100 GeV ), we see that it is in good agreement with the predictions from the other approaches. However, as higher values of $H_{T}$ are probed, the Hes prediction becomes noticeably larger than the fixed-order descriptions, including those from SHERPA where different multiplicities are merged. This is the region in $H_{T}$ where we would expect high multiplicities to have a noticeable effect, and therefore where we would expect to see the impact of the resummation in Hej. This is, however, slighlty at odds with the fact that the SHERPA prediction included up to 6 jets and that the multijet rates and the $p_{\perp}$ distributions of the fifth and sixth jet from HeJ undershoot those from SHERPA, cf. Fig. 93


Fig. 92: $H_{T}=\sum_{i \in\{\mathrm{jets}\}} E_{\perp i}$ of events with at least 2 jets on all levels of the simulation (for exact definitions and cuts see App. 18.61 and App. 18.62. Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).
and Fig. 95. However, a similar trend concerning the hard tail of this distribution appears also on the shower level in the MadGraph+Pythia sample, which includes up to 4 extra jets, and in the Powheg Box + PYthia8 sample, which includes 2 jets at LO and 1 jet at NLO. The trend is even more pronounced with an even harder tail for the PYTHIA8 MEPS sample, which includes 3 extra jets. At this level, SHERPA more or less follows the NLO result. It should be noted, though, that all approaches remain within the scale variation band indicated on the BlackHat prediction. This findings are consistently carried over to the hadron and hadron+MPI level.

Turning to the $n$-jet rates, at the matrix element level, SHERPA follows fairly closely the NLO results in different jet multiplicity bins, while HeJ seem to overshoot the central value in the 3-and 4-jet bin, but staying inside the NLO scale uncertainty band. going back to the tree-level result of SHERPA in the 5- and 6-jet bins. As discussed in Sec. 18.33, the HeJ framework includes tree-level matching for final states with up to and including four jets in the final state. Therefore it is fair to assume that the absence of matching for five jets and above leads to the larger drop in cross section observed in Fig. 93 from four-jet to five-jet as compared to that from either three-jet to four-jet or from five-jet to six-jet and lends support to the suspicion that in HEJ a matched sample would also provide larger 5- and 6-jet multiplicities. At the shower level, the trend already visible at the $H_{T}$ distribution repeats itself. The smaller cross section in the PYTHIA8 MEPS sample is mainly due to the low multiplicity bins, such that the shape of the $n$-jet distribution also has a relatively harder tail than the SHERPA sample. In contrast,


Fig. 93: Number of jets on all levels of the simulation (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that Powheg Box+Pythia8 and GoSam calculate $W+1$ jet on matrix element level, while Hej starts with $W+2$ jets and that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).
the Powheg Box +Pythia8 result, starting consistently at 1 jet, appear to be at the upper end of the NLO uncertanities throughout.

Looking at the correlation of the two leading jets in Fig. 94 at the matrix element only, both the $\Delta R$ and the $m_{12}$ distribution provided by SHERPA have a slight tilt against the NLO prediction from BLACKHAT+ SHERPA, undershooting the latter result by up to about $40 \%$ for large $\Delta R$ and by up to about $20 \%$ for large $m_{12}$. While HEJ seems to roughly follow the shape of SHERPA for $\Delta R$, it is significantly harder than SHERPA and the NLO result for large values of $m_{12}$. In addition, in both cases, HeJ also predicts a larger cross section that the other tools.

Fig. 95 shows the transverse momentum distributions for the third to sixth jets ordered in $p_{\perp}$, and at the matrix element level. For the third hardest jet, the prediction from HEJ is similar in shape but higher in cross section than the results obtained at NLO from BLACKHAT+SHERPA or the two SHERPA samples. For the fourth jet, the Hej cross section still seems higher than the other ones, but this discrepancy seems to be mainly around comparably low jet $p_{\perp}$. For larger values of $p_{\perp}$ all tree-level type or resummed predictions are below the NLO result. Surprisingly, for the fifth and sixth hardest jets, the HEJ predictions follow the SHERPA ones for low values of $p_{\perp}$ below about 60 GeV , before they fall off nearly instantly. This again may be an artefact of tree-level matching not being included in HeJ for the production of fiveand six-jets or of missing statistical support in this region of phase space.


Fig. 94: $\Delta R$ of two leading jets (left) and invariant mass of two hardest jets (right) matrix element level (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).


Fig. 95: Transverse momentum of third to sixth hardest jet on matrix element level (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, PYTHIA8 and MadGraph+PyTHIA CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BlackHat+Sherpa (on matrix element level).

### 18.5 Conclusions

In this study first steps towards an update and extension of the comparison in [439] have been made. In contrast to the older study, a larger variety of tools including fixed-order and resummation tools as well as NLO matched and tree-level merged simulations have been included. Not surprisingly, some observables appear to be described fairly consistently between different tools, while others exhibit large deviations, sometimes clearly beyond the formal accuracy claimed by the different methods, and also beyond the best estimates of intrinsic modelling or calculational uncertainties provided by the authors. In some instances the relative differences are way beyond naïve expectations by most of the authors of this study. This clearly hints at the need to carefully cross-validate different tools before deploying them for large scale simulations, and it also necessitates an increased collaboration of the authors of such tools in order to arrive at a more consistent picture.

We hope that this study triggered some future work towards the latter goal.

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### 18.6 Cuts and observables

### 18.61 Cuts

|  | ATLAS | CMS |
| :--- | :--- | :--- |
| lepton $p_{\perp}$ | $>20 \mathrm{GeV}$ | $>20 \mathrm{GeV}$ |
| lepton $\|\eta\|$ | $<2.5(e, \mu)$ | $<2.5(e), 2.1(\mu)$ |
| $\mathbb{E}_{\perp}$ | $>25 \mathrm{GeV}$ | no cut |
| $m_{\perp, W}$ | $>40 \mathrm{GeV}$ | $>20 \mathrm{GeV}$ |
| jet $p_{\perp}$ | $>25 \mathrm{GeV}$ | $>30 \mathrm{GeV}$ |
| jet $\|\eta\|$ | $<4.4$ | $<2.4$ |
| jet radius | $0.4\left(\right.$ anti- $\left.k_{\perp}\right)$ | $0.5\left(\right.$ anti- $\left.k_{\perp}\right)$ |
| lepton isolation | $<10 \%$ of lepton energy | $<10 \%$ of lepton energy |
|  | in cone with R=0.5 | in cone with R=0.5 |

Table 13: Cuts used in this study inspired by common ATLAS and CMS cuts.

Tab. 13 presents the cuts applied to define the event selection in both the ATLAS and CMS specifications.

### 18.62 Analysis procedure and definition of observables

A common analysis was implemented within the RIVET framework and used by all codes providing individual events. This analyses is carried out as defined in the following:

1. remove all neutrinos from all final states (i.e. 'all particles' from now on means 'all particles without neutrinos')
2. find hardest isolated lepton (electron or muon) ('lepton' from now on means 'hardest isolated lepton')
3. cut on lepton $p_{\perp}$ and $|\eta|$
4. compute missing transverse energy $E_{\perp}$ :
(a) sum the three-momenta of all particles within $|\eta|<10$, this yields $-\not p$
(b) compute missing energy as $\notin=|\boldsymbol{p}|$
(c) assume resulting four-vector $\not p$ corresponds to neutrino
5. for ATLAS cut on $E_{\perp}$
6. resonstruct $W$ four-momentum as $p^{W}=p^{\text {lepton }}+\not p$
7. compute $W$ transverse mass squared as $m_{\perp, W}^{2}=\left(p_{\perp}^{\text {lepton }}+\not p_{\perp}\right)^{2}-\left(p_{\perp}^{W}\right)^{2}$
8. cut on $W$ transverse mass
9. remove lepton from final state
10. cluster into jets keeping only those passing the $p_{\perp}$ and $|\eta|$ cuts
11. compute $H_{T}=\sum_{i \in\{\text { jets }\}} E_{\perp i}$
12. compute beam thrust $\tau_{B}=\sum_{i \in\{\text { particles }\}}\left(E_{i}-\left|p_{i}^{z}\right|\right)$ using all visible particles

It should be noted that this defintion of the $W$ is infra-red safe only for transverse observables.

### 18.7 Detailed settings

### 18.71 Sherpa

For this study Sherpa-1.3.1 was used. Except for the underlying event, which was tuned for the CT10 [255] parton distribution functions and whose parameters are given below, all other nonperturbative parameters were kept at their default values. The underlying model was tuned for the cluster hadronisation.

| K_PERP_MEAN_1 | 1.17 |
| :--- | :--- |
| K_PERP_MEAN_2 | 1.17 |
| K_PERP_SIGMA_1 | 0.760 |
| K PERP_SIGMA_2 | 0.760 |
| PROFILE_PARAMETERS | $0.576,0.353$ |
| RESCALE_EXPONENT | 0.238 |
| SCALE_MIN | 2.52 |
| SIGMA_ND_FACTOR | 0.465 |

### 18.72 Pythia8

To produce the results, we have used two tunes of Pythia8, Tune 4C and Tune A2, both of which use CTEQ6L1 parton distributions. Tune 4C is the default tune in PYTHIA8- no additional input settings are necessary. For completeness, below we list all parameters that are implicitly set by choosing the default Tune 4C.

```
PDF:pSet = 8
SigmaProcess:alphaSvalue = 0.135
SigmaDiffractive:dampen = on
SigmaDiffractive:maxXB = 65.0
SigmaDiffractive:maxAX = 65.0
SigmaDiffractive:maxXX = 65.0
```

```
TimeShower:dampenBeamRecoil = on
TimeShower:phiPolAsym = on
SpaceShower:alphaSvalue = 0.137
SpaceShower:samePTasMPI = false
SpaceShower:pT0Ref = 2.0
SpaceShower:ecmRef = 1800.0
SpaceShower:ecmPow = 0.0
SpaceShower:rapidityOrder = on
SpaceShower:phiPolAsym = on
SpaceShower:phiIntAsym = on
MultipartonInteractions:alphaSvalue = 0.135
MultipartonInteractions:pT0Ref = 2.085
MultipartonInteractions:ecmRef = 1800.
MultipartonInteractions:ecmPow = 0.19
MultipartonInteractions:bProfile = 3
MultipartonInteractions:expPow = 2.0
BeamRemnants:primordialKTsoft = 0.5
BeamRemnants:primordialKThard = 2.0
BeamRemnants:halfScaleForKT = 1.0
BeamRemnants:halfMassForKT = 1.0
BeamRemnants:reconnectRange = 1.5
```

A detailed discussion of these choices can be found in [455]. All other parameters remain with their default values. For our purposes, it might be interesting to remark that the starting value for $\alpha_{s}$-evolution in time-like splittings is given by

SpaceShower:alphaSvalue $=0.1383$
To investigate the impact of rapidity ordering in space-like showers, we chose to remove enforced rapidity ordering by setting

SpaceShower:rapidityOrder = off
If rapidity ordering is enforced in ISR, the question arises how it should be treated when picking histories. For this purpose, PYTHIA8 supplies the switch

Merging:enforceStrongOrdering
When switched "on", this parameter will result in picking non-rapidity-ordered histories only if no rapidity-ordered paths where found, thus disfavouring non-rapidity-ordered parton shower histories for matrix element states. To have a more complete understanding of the impact of tuning, we also changed to the recently proposed Tune A2 [458]. For this, we have to set

Tune:pp $=7$
Pythia8 will then reset the following parameters:

```
PDF:pSet = 8
SigmaProcess:alphaSvalue = 0.135
SigmaDiffractive:dampen = on
SigmaDiffractive:maxXB = 65.0
SigmaDiffractive:maxAX = 65.0
```

```
SigmaDiffractive:maxXX = 65.0
TimeShower:dampenBeamRecoil = on
TimeShower:phiPolAsym = on
SpaceShower:alphaSvalue = 0.137
SpaceShower:samePTasMPI = false
SpaceShower:pT0Ref = 2.0
SpaceShower:ecmRef = 1800.0
SpaceShower:ecmPow = 0.0
SpaceShower:rapidityOrder = false
SpaceShower:phiPolAsym = on
SpaceShower:phiIntAsym = on
MultipartonInteractions:alphaSvalue = 0.135
MultipartonInteractions:pTORef = 2.18
MultipartonInteractions:ecmRef = 1800.
MultipartonInteractions:ecmPow = 0.22
MultipartonInteractions:bProfile = 4
MultipartonInteractions:a1 = 0.06
BeamRemnants:primordialKTsoft = 0.5
BeamRemnants:primordialKThard = 2.0
BeamRemnants:halfScaleForKT = 1.0
BeamRemnants:halfMassForKT = 1.0
BeamRemnants:reconnectRange = 1.55
```

Apart from not enforcing rapidity ordering in space-like splittings, this tune differs from Tune 4C in that the proton size is considered $x$-dependent. This is in the spirit of Tune $4 C X$, which was introduced in [470]. In general, since we include matrix element states for two and three jets, we do not apply additional matrix element corrections in PYTHIA8 after the first emission, by setting

```
SpaceShower:MEafterFirst = off
TimeShower:MEafterFirst = off
```


### 18.73 Powheg Box + PYtHiA8

For this study we used Powheg Box rev1282 and Pythia 8.153. Except for the specific subprocess requested, the parton distribution functions set and the renormalisation/factorisation scale factors chosen, all the other parameters were kept fixed below during all the runs. Here is a sample Powheg Box input file:

```
! W^+ + jet production parameter
idvecbos 24 ! PDG id of vector boson (24: W+, -24: W-)
vdecaymode 1 ! decay channel (1: electron, 2: muon, 3: tau)
numevts 4000000 ! number of events to be generated
ih1 1 ! hadron 1 (1 for protons, -1 for antiprotons)
ih2 1 ! hadron 2 (1 for protons, -1 for antiprotons)
ebeam1 3500d0 ! energy of beam 1 in GeV
ebeam2 3500d0 ! energy of beam 2 in GeV
lhans1 192800 ! pdf set for hadron 1 (LHA numbering)
lhans2 192800 ! pdf set for hadron 2 (LHA numbering)
ncall1 100000 ! number of calls for initializing the ...
itmx1 5 ! number of iterations for initializing the ...
ncall2 250000 ! number of calls for computing the integral ...
```

| itmx2 | 4 | ! number of iterations for computing the ... |
| :--- | :--- | :--- | :--- |
| foldcsi | 1 | ! number of folds on csi integration |

When interfacing to Pythia8 we have changed the following settings with respect to Pythia8 defaults, for the various stages under investigations:
///Hadron Level w MPI and QED
BeamRemnants:reconnectRange $=1.50000$
MultipleInteractions:alphaSvalue $=0.13500$
MultipleInteractions:bProfile = 3
MultipleInteractions:ecmPow $=0.1900$
MultipleInteractions:expPow $=2.0000$
MultipleInteractions:pT0Ref $=2.0850$
PDF:pSet $=8$
SigmaDiffractive:dampen $=$ on
SigmaDiffractive:maxAX $=65.0000$
SigmaDiffractive:maxXB $=65.0000$
SigmaDiffractive:maxXX $=65.0000$
SigmaProcess:alphaSvalue $=0.13500$
SpaceShower:MEafterFirst $=$ off
SpaceShower:MEcorrections = off
SpaceShower:pTmaxMatch $=0$
SpaceShower:rapidityOrder = on
TimeShower:MEcorrections $=$ off
TimeShower:MEafterFirst $=$ off
TimeShower:pTmaxMatch $=0$
//Hadron Level w MPI (added)
SpaceShower:QEDshowerByQ = off
SpaceShower:QEDshowerByL = off
TimeShower:QEDshowerByQ $=$ off
TimeShower:QEDshowerByL $=$ off
//Hadron Level w/o MPI (added)
PartonLevel:MI = off

```
//Shower Level (added)
HadronLevel:All = off
//Parton Level (added)
PartonLevel:ISR = off
PartonLevel:FSR = off
PartonLevel:Remnants = on
```

and, most important, we have vetoed shower emissions with a transverse momentum greater than the value of SCALUP read from the Les Houches event file for the corresponding event.

### 18.74 MADGRAPH + PYTHIA

For this study MADGRAPH/MADEVENT 5.1.1.0 and Pythia 6.4.2.4 is used. The LHE files are generated for events with a $W$ and up to four additional partons, i.e. for the process:

```
pp>w- -> l-vl~ ; l-vl~~j ; l-vl~~jj ;l-vl~~jjj ; l-vl~~jjjj ;
l-vl~ ; l-vl~j ; l-vl~jj ;
l-vl~jjj ; l-vl~ jjjj ()
```

The mass of the b quark is set to zero. The strong constant $\alpha_{s}\left(M_{Z}^{2}\right)$ is set to 0.1300 both in the matrix element calculation and in the proton PDF, that is the CTEQ6L1.

Pythia is used for the parton shower and the hadronisation with the following parameters modified according to tune Z 2 .

```
MSTU(21)=1 ! Check on possible errors during program execution
MSTJ(22)=2 ! Decay those unstable particles
PARJ (71)=10 . ! for which ctau 10 mm
MSTP(33)=0 ! no K factors in hard cross sections
MSTP(2)=1 ! which order running alphaS
MSTP(51)=10042 ! structure function chosen (external PDF CTEQ6L1)
MSTP(52)=2 ! work with LHAPDF
PARP(82)=1.832 ! pt cutoff for multiparton interactions
PARP(89)=1800. ! sqrts for which PARP82 is set
PARP(90)=0.275 ! Multiple interactions: rescaling power
MSTP(95)=6 ! CR (color reconnection parameters)
PARP (77)=1.016 ! CR
PARP (78)=0.538 ! CR
PARP (80)=0.1 ! Prob. colored parton from BBR
PARP(83)=0.356 ! Multiple interactions: matter distribution para...
PARP(84)=0.651 ! Multiple interactions: matter distribution para...
PARP (62)=1.025 ! ISR cutoff
MSTP(91)=1 ! Gaussian primordial kT
PARP(93)=10.0 ! primordial kT-max
MSTP(81)=21 ! multiple parton interactions 1 is Pythia default
MSTP (82)=4 ! Defines the multi-parton model
PMAS (5,1)=4.8 ! b quark mass
PMAS (6,1)=172.5 ! t quark mass
MSTJ(1)=1 ! Fragmentation/hadronization on
MSTP(61)=1 ! Parton showering on
```

For additional studies, we set

```
MSTJ(41)=3 ! switch off lepton FSR
MSTP(81)=20 ! switch off MPI
MSTJ(1)=0 ! Fragmentation/hadronization off
```

to switch off, respectively, final state QED radiation, multi-particle interactions, and hadronisation.

## Part V

## EXPERIMENTAL DEFINITIONS AND CORRECTIONS

## 19. PHOTON ISOLATION AND FRAGMENTATION CONTRIBUTION ${ }^{43}$


#### Abstract

Photon isolation and its link with the fragmentation contribution is explored via NLO matrix-element generator and parton-shower Monte-Carlo.

Firstly the dependence of the inclusive photon and di-photon NLO cross sections to the choice of isolation criteria are investigated. The isolation criteria used is the discretized version of the Frixione isolation, with parameters chosen for those most practical at an experimental level. As an extention, a more generalized version of the standard Frixione isolation is also studied. The selection of scale is also investigated in search of the 'saddle point', which would give the optimal scale choice. In addition the choice of jet algorithm is investigated for the photon with associated jet cross section. Secondly, properties of the fragmentation contribution in parton-shower Monte-Carlos are investigated. The distance profile of the photon to the other generator level particles in the event is explored in the case of neutral mesons, fragmentation photons and direct photons. Next the impact of a "hollow" or "crown" isolation criterion, expected to enhance the fragmentation contribution, is explored. Then, to complement the NLO inclusive studies, the impact of typical Frixione isolation criteria on the fragmentation component are investigated in the parton-shower Monte-Carlos.


Finally conclusions are made comparing the properties of the fragmentation contribution in NLO generators and parton-shower generators.

### 19.1 INTRODUCTION

Experimental measurements of single photons and di-photons require the application of isolation cuts to reduce the copious backgrounds arising from jet fragmentation. Such cuts also have the impact of reducing the fragmentation contributions of photon production. On the theoretical side, including fragmentation contributions of photon production can greatly increase the complexity of the calculations, while the application of appropriate isolation cuts can effectively remove those fragmentation contributions.

[^152]
### 19.11 Frixione isolation

In the following we will study the Frixione isolation criterion [471], which was designed to suppress the fragmentation contribution. It has been shown to reduce the fragmentation contribution in NLO generators [18]. The question is to know whether or not the behavior is still applicable using parton shower Monte-Carlo and if it can be used experimentally.

We consider the following function for the isolation criterion :

$$
\begin{equation*}
E_{T}^{i s o}(R)<f(R)=\epsilon \cdot p_{T, \gamma} \cdot\left(\frac{1-\cos (R)}{1-\cos \left(R_{0}\right)}\right)^{n} \tag{19.1.1}
\end{equation*}
$$

where $E_{T}^{i s o}(R)$ is the isolation sum of all particles inside a cone of $R=\sqrt{\Delta \phi^{2}+\Delta \eta^{2}}$ around the photon, $\epsilon$ is the strength or the scale of the isolation criterion, $p_{T, \gamma}$ is the transverse energy of the photon, $R_{0}$ is the first considered cone and $n$ the power of the isolation criterion. This formula can be altered by replacing $p_{T, \gamma}$ with a fixed threshold. Functional forms $f(R)$ for different $\epsilon$ and $n$ are shown Fig. 96


Fig. 96: Examples of Frixione functional form for different parameters.

The Frixione isolation is tighter and tighter when decreasing the $R$ cone size. With matrix element NLO generators (as in Jetphox [472, 473] and Diphox [474]), the only contribution possible at a given $R \neq 0$ is the one coming from the suplementary hard jets in the event, while the fragmentation debris are emitted colinearly to the photon at $R=0$ (angle information is lost due to the fragmentation function which is integrated over the angle). With parton-shower generator, fragmentation photons are emitted off quarks at a non-zero angle during the showering process. In the following sections we will study the link between isolation and fragmentation in NLO generators, then with parton-shower Monte-Carlo.

### 19.12 Experimental complications

There are various mismatches between isolation cuts applied to theoretical calculations and isolation cuts applied to data (or to Monte Carlo). First of all, we wish to apply the isolation cut only to energy related to the hard scatter. Experimentally, most of the energy inside an isolation cone is due to the underlying event associated with the hard scatter, or the remnants of additional interactions in the same crossing. Techniques such as jet area subtraction [475, 476] can be used to remove an amount of energy from the isolation cone roughly equal to the expected contamination from underlying event/pileup, leaving only energy related to the hard scatter and specifically to fragmentation processes. Since there is no underlying event/pileup in partonic level theory calculations, only the isolation cut needs to be applied to the theory.

Full details of the use of this correction within the ATLAS collaboration can be found in the inclusive cross section measurement [477]. The ATLAS isolation definition uses a cone around the cluster of cells that are identified as a photon. These photon cluster cells are not included in the sum, so there is first a correction for any leakage of the photon shower into the surrounding cells (typically a few percent of the photon $p_{T}$ ). The pile-up/underlying event correction is then applied by calculating per event the ambient energy from the jet activity in that specific event. This follows the jet area corrections method mentioned above, where all jets are reconstructed without any minimum momentum threshold. The energy density of each jet is calculated and the median density is used for the correction. In 2010 this typically resulted in a correction of around 900 MeV .

The original Frixione isolation scheme assumed that an isolation cut could be applied continuously as a function of R (distance from the photon). Actual detectors have a finite granularity. A solution to this was the adoption of a discretized version of Frixione isolation, allowing this granularity to be taken into account [18]. However, it is not possible to place an isolation cut on the inner-most cone (typically $R \sim 0.1$ ), because of the presence of the photon itself. While the separation between the fragmentation photon and the jet remnants is finite in data (and in Monte Carlo), fragmentation is treated as a collinear process in partonic cross sections. The inability to apply the isolation cut down to $R=0$, results in a greatly reduced ability to discriminate against fragmentation processes in the partonic level theory.

To rectify this the Frixione calculation could be modified into a 'crown' isolation, whereby the last cone is missed from the calculation. Unfortunately as most of the radiation is collinear in the fragmentation events, it is likely to reduce its effect of removing these events. Other studies [478] have shown that the photon quality cuts applied by the experiments will reduce the fraction of fragmentation photons accepted, where substantial fragmentation energy is collinear with the photon. However, the rejection is not $100 \%$, so we are still left with a smaller reduction of fragmentation contributions in the partonic level theory than are actually (presumably) present in the data. In these proceedings, we will discuss how to more properly incorporate the correct level of rejection in the theory.

### 19.13 Choice of fragmentation scale

In addition to the experimental difficulties with applying the isolation criteria there are also difficulties in choosing appropriate scales for the theoretical calculation. This is discussed in the following text, along with other considerations for applying Frixione isolation at a theoretical level.

Fragmentation is treated as a collinear process in partonic calculations. In this framework, the original "continuous" Frixione criterion [471] was designed to inhibit the appearance of final state photonparton collinear singularities which otherwise require absorption in a fragmentation function $D\left(z, M_{F}\right)$. Thus, cross sections for the production of prompt photons isolated with this criterion involve no fragmentation contribution. Discretized variants of this criterion have been proposed which aim at matching better what can be actually implemented experimentally [18]. They consist in a limited number of nested cones $\mathcal{C}_{j=1, \cdots, n}$ with respective radii $R_{1}=R_{\min }<R_{2}<\cdots<R_{n}=R_{\max }$ defined in the azimuthal and rapidity differences with respect to the photon direction, and requiring recursively that the accompanying hadronic transverse energies inside every successive cone $\mathcal{C}_{j}$ be less than an ordered sequence of maximum values ${ }^{44} E_{T j}^{i s o}$ such that $0<E_{T 1}^{i s o}<\cdots<E_{T n}^{i s o}$. However, in contrast with the continuous criterion, such discretized variants still involve a fragmentation contribution, though the latter is expected to be small, since the situation in the innermost cone shares some similarity with the standard cone criterion. When quantifying the magnitude of the fragmentation contribution with such discretized criteria, a potentially tricky issue concerns the fragmentation scale dependence and the "best choice" of scale.

This issue matters for isolation with the standard cone criterion when the radius $R$ of the cone is $\ll 1$ while $E_{T}^{i s o}$ is kept fixed. Whereas the natural fragmentation scale $M_{F}$ in the non-isolated case

[^153]is $\sim p_{T}^{\gamma}$, this choice can lead to very poor theoretical estimates at Next to Leading Order (NLO) in perturbative QCD when $R \ll 1$ [472]. The scale dependence near the choice $M_{F} \sim p_{T}^{\gamma}$ is then large and, worse, the theoretical prediction may eventually exhibit an unphysical violation of unitarity whereby the predicted NLO cross section for photons becomes larger than the inclusive one, so that even for only moderately small $R$ the reliability of the prediction is questionable. On the other hand, as ${ }^{45} D\left(z, M_{F}\right) \sim$ $\log \left(M_{F} / \Lambda_{Q C D}\right)$, with the choice $M_{F} \sim R p_{T}^{\gamma}$ the fragmentation contribution is suppressed compared with $M_{F} \sim p_{T}^{\gamma}$. The situation is improved regarding both scale dependence and unitarity, although it does not solve the problem completely. One actually faces a multiscale problem: $\Lambda_{Q C D} \ll R p_{T}^{\gamma} \ll p_{T}^{\gamma}$, and a one-scale compromise is possibly insufficient depending on the kinematical regime explored. The atypical choice $M_{F} \sim R p_{T}^{\gamma}$ has in principle to be supplemented by a resummation of the logarithmic $R$ dependence coming form outside the cone, if at all possible. At leading-log $R$ (LLR) accuracy at least, such a resummation is actually feasible, which furthermore allows to solve the apparent puzzle why scale choices should be very different in the cases with isolation in a narrow cone vs. broad cone or without isolation.

The concern about the discretized Frixione criteria is that the innermost cone size is quite small. The choice for the fragmentation scale $M_{F}$ shall then arguably be $M_{F} \sim \mathcal{O}\left(R_{\min } p_{T}^{\gamma}\right)$. On the other hand, as the allowed transverse energy deposit $E_{T}^{i s o}\left(R_{\text {min }}\right)$ inside this cone is correspondingly small, the width of the interval in the fragmentation variable on which the fragmentation function is convoluted with the partonic cross section is restricted to a rather narrow range $0<1-z<E_{T}^{i s o}\left(R_{\min }\right) / p_{T}^{\gamma} \sim$ $\epsilon\left(R_{\min } / R_{\max }\right)^{n}$. This leads to a quite suppressed fragmentation contribution. The combination of the two effects: a low fragmentation scale and a narrow $z$-range, is the discrete counterpart of the inhibition of fragmentation by the continuous criterion. We may thus expect that the issue of the narrow cone is less worrying for the reliability of the NLO calculation in this case than if only $R$ were taken small while keeping $E_{T}^{i s o}$ fixed. In order to assess the uncertainty on the fragmentation contribution we may perform the calculation for the "arguably better" scale $M_{F} \sim R_{\min } p_{T}^{\gamma}$ and compare it to the expectedly larger result for the standard choice $M_{F} \sim p_{T}^{\gamma} / 2$.

### 19.2 ISOLATION FOR INCLUSIVE PHOTONS AND DIPHOTONS AT NLO

The study at NLO uses the Jetphox generator to calculate the inclusive photon cross section and Diphox for the di-photon cross section. Details of how to use the software and to obtain predictions with errors can be found in [480] and the selection criteria used are listed in the appendix. Previous results from Les Houches [18] showed that the discretized Frixione isolation criteria did manage to reduce the fragmentation contribution, here we extend that study in several ways. Firstly the cross section returned has been compared to that calculated from using the standard cone isolation, as used in current measurements. A generalized form of the Frixione isolation is discussed, aimed to satisfy both the experimental and the theoretical requirements on the isolation cut for different $p_{T}$ regimes. In addition the effects of changing the number of cones used in the calculation and of choosing an $E_{T}$ cut, rather than relating it to the photon $p_{T}$, are investigated. In addition, further complications to comparing theoretical and experimental isolation calculations are discussed. Finally there are further brief studies using Jetphox to look at scale and jet algorithm choices.

### 19.21 Discretized prescription

The parameters used to define different selections, according to Eq. 19.1.1, were:

$$
\begin{array}{llll}
a: \epsilon=0.05 n=0.2 & b: \epsilon=1 n=0.2 & c: \epsilon=1 n=1 & d: \epsilon=0.5 n=1 \\
e: \epsilon=0.05 n=1 & f: \epsilon=1 n=0.1 & g: \epsilon=1 n=0.5 &
\end{array}
$$

[^154]

Fig. 97: Left: Fragmentation fraction for the cone and Frixione isolation criteria. Right: The applied $E_{T}$ cut on the isolation sum as a function of $p_{T}$ for the 0.4 cone or 0.1 cone in the Frixione criteria.
where all but the last two were based on the previous study. In all cases $R_{0}$ was chosen to be 0.4 , with $R$ being set to either: $0.4,0.3,0.2,0.1$ or $0.4,0.35,0.3,0.25,0.2,0.15,0.1$.

The comparison to the cone isolation in Fig. 97 shows that out of the chosen parameters only 1 set removes the fragmentation contribution more than what is removed by the cone algorithm, although two are lower until high $p_{T}$. It also shows that criteria $b$ and $f$ are not much better than applying no isolation criteria at all. When altering Eq. 19.1 .1 to use a fixed $E_{T}=4 \mathrm{GeV}$ instead of $p_{T, \gamma}$ the results are more promising but this is because it applies a cut in the 0.1 cone that is below the experimental accuracy (of the order 100 MeV due to detector resolution/noise). Unfortunately Fig. 97 also shows that this is also the case for the $p_{T}$ requirements, as case $e$ (the only criteria to perform better than the standard cone) also applies a cut that is not viable experimentally in the 0.1 cone.

There are some positive outcomes from these studies, firstly the Frixione criteria $b$ and $d$ maybe useful criteria to use experimentally as they keep the fragmentation contribution similar and low in all bins, which could help with understanding of the systematic errors/correlation between bins. Secondly the comparison of the number of cones used in the Frixione criteria resulted in a difference of around $1 \%$ on the total cross section and almost no effect on the fragmentation fraction. This means that it is fine to use the lower number of cones case, and that the discrete Frixione criteria is most likely very similar to that of the continuous version.

### 19.22 Generalized prescription

As seen previously, to remove the fragmentation contribution in the theory, a small value of $\varepsilon$ is needed. However, given the effects of finite resolution and granularity on the experimental description of the isolation energy, a minimum threshold has to be allowed in the isolation cone, especially at low $p_{T}$. A typical value of $2-4 \mathrm{GeV}$ is used as experimental cut, to optimize the rejection of hadronic background coming from the decay of light mesons. Now, at high $p_{T}$ this cut might result too tight, particularly on the theoretical side given that an isolation cut much smaller than the photon $p_{T}$ can cause large logs in the calculations, this effect was not observed in the previous Les Houches study.

As a good compromise of these two requirements, it has been proposed [481] to extend the original


Fig. 98: Effect of the two terms in the modified Frixione isolation prescription effects of the different pieces of the generalized Frixione isolation prescription on the isolation cut as a function of $p_{T}$ (left) and the cone radius R (right).

Frixione prescription (Eq. 19.1.1) to a more general form:

$$
\begin{equation*}
E_{T}^{i s o}<\left(\left(E_{0}\right)^{k}+\left(\varepsilon \cdot p_{T}\right)^{k}\right)^{1 / k}\left(\frac{1-\cos R}{1-\cos R_{0}}\right)^{n} \tag{19.2.1}
\end{equation*}
$$

where:
$R_{0}$ is the maximum cone size
$E_{0}$ is the minimum energy pedestal allowed in a cone of size $R_{0}$
$\varepsilon$ is the fraction of the photon $p_{T}$ allowed in the cone of size $R_{0}$
$k$ determines the shape of the isolation profile in $p_{T}$
$n$ determines the shape of the isolation profile in R (see Fig. 98 right])
The extra parameters give enough flexibility to ensure a (finite) tight cut at low $p_{T}\left(\sim E_{0}\right)$ and, at the same time, a loose cut at high end of the spectrum driven by the photon $p_{T}$. The $k$ parameter controls how quickly/smoothly is the transition from one regime to the other (see Fig. 98 left]).

This generalized prescriptior ${ }^{[46}$ has been implemented in Jetphox recently and some possible configurations are explored here. The studied configurations vary $\varepsilon(=0.05,1)$ and $k(=2,5,10)$, and have a fixed value for $E_{0}=4 \mathrm{GeV}$ (the typical cut applied in ATLAS) and $n=0.5$ (given the linear behaviour of isolation distribution width observed for direct photons in ATLAS [482]).

The high- $\varepsilon$ configurations ( $\varepsilon=1$ ), show a worse performance at removing the fragmentation contribution with respect to the fixed cone approach and are practically insensitive to the value of $k$ in the formula. The remaining fragmentation fraction is $\sim 25 \%$ at 45 GeV decreasing to $20 \%$ in the highest $p_{T}$ bin. On the other hand, as seen in Fig. 99, all the configurations for a low value of $\varepsilon(=0.05)$ show an improvement in fragmentation rejection compared to both the no isolation and fixed cone cases, in the whole $p_{T}$ region ( $45 \mathrm{GeV}<\mathrm{p}_{\mathrm{T}}<600 \mathrm{GeV}$ ). The $p_{T}$ profile for the smaller cone ( $R=0.1$ ) in this case (Fig. 99[right]) looks also more promising in terms of its applicability at the experimental level.

[^155]

Fig. 99: Left: Fragmentation fraction for the cone and the (generalized) Frixione isolation criteria. Right: The applied isolation cut as a function of $p_{T}$ for 0.1 cone in the (generalized) Frixione criteria.

### 19.23 Continuous and discretized Frixione criteria in di-photon events

Following the previous studies with inclusive photons, we now consider the production of photon pairs. The aims of this study are i) to assess the effect on the magnitude of the fragmentation contribution by comparing results from using the continuous Frixione criterion with those using several variants of the discretized version, implemented in the NLO programme Diphox, thereby providing a NLO assessment of how much fragmentation may be missing in the NNLO calculation of Catani et al. [78] which includes no fragmentation and therefore uses the continuous criterion; ii) to probe the dependence of the prediction with respect to the fragmentation scale choice. It supplements a similar comparison which had been performed for inclusive photon production in [18].

Fig. 100 provides a comparison of the original continuous criterion to the discretized version of the criterion based on four nested cones with respective radii $R_{\text {min }}=0.1, R_{2}=0.2, R_{3}=0.3$ and $R_{\max }=0.4$. Four variants of the energy profile $E_{T}^{\text {iso }}(R)$ as defined in Eq. 19.1.1 have been considered: $(\epsilon, n)=(0.05,0.2),(0.05,1),(0.5,1)$ and $(1,1)$. Fig. 100 (left) presents the distribution in invariant mass of photon pairs in the range $40 \mathrm{GeV} \leq m_{\gamma \gamma} \leq 300 \mathrm{GeV}$. The discretized criterion $(0.05,1)$ suppresses fragmentation so much that there is practically no difference between the discretized and continuous versions. With the criterion $(1,1)$, the discretized version leads to a distribution $O(10-12 \%)$ larger than the continuous one. The choice $(0.5,1)$ displays a similar feature, though quantitatively less important. The energy profile of the fourth choice is not suited for an efficient isolation unless $\epsilon$ is chosen very small. A similar comparison is shown on Fig. 100 (right) for the distribution in the difference in azimuthal angle $\Delta \phi$ between the two photons. Whereas the distribution in invariant mass is dominated by the direct contribution, the tail of the distribution in $\Delta \phi$ tail at low $\Delta \phi$ is more sensitive to the fragmentation contribution. Therefore, the conclusions are qualitatively similar to the one drawn for the distribution in invariant mass, yet the effects are quantitatively larger.

Fig. 101 assesses the dependence on the fragmentation scale $M_{F}$, for the distributions in invariant mass (left) and in $\Delta \phi$ (right) respectively. Two choices were considered: $M_{F}=R_{\min } \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}=$ $0.1 \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}$ vs. $M_{F}=R_{\max } \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}=0.4 \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}$ closer to a standard choice ${ }^{47}$. As expected, the distribution in invariant mass, which is not very sensitive to the fragmen-

[^156]

Fig. 100: Comparing continuous and discretized Frixione criterions for the distributions in $m_{\gamma \gamma}$ (left) and $\Delta \phi$ (right) of photon pairs, for four variants of the criterion.


Fig. 101: Fragmentation scale dependence of the distribution in $m_{\gamma \gamma}$ (left) and $\Delta \phi$ (right) of photon pairs, for four variants of the discretized Frixione criterion.
tation contribution, is practically not impacted by the choice. The distribution in $\Delta \phi$ is more sensitive to the fragmentation component and the sensitivity to the fragmentation scale choice is larger than for the distribution in invariant mass. The sensitivity to the fragmentation scale choice is the largest in the case of the criterion $(\epsilon, n)=(1,1)$, for which the predictions are $5-7 \%$ smaller, rather uniformly, with the lower scale choice than with the more standard one.

In conclusion this preliminary study shows that the impact of the fragmentation contribution passing the discretized criterion seems to be almost negligible on the distribution in invariant mass, and remains small even on the tail of the distribution in azimuthal angle. Notwithstanding, the conclusions shall have limited use depending on how isolation is actually implemented experimentally in the innermost cone. We here stick to a discretized version of the Frixione criterion which respects the original idea of a transverse energy deposit decreasing towards zero with the cone radius. If instead any experimental constraint would allow a more permissive condition in the innermost cone, a dedicated study would be mandatory.

### 19.24 Additional studies at NLO

In addition to the isolation studies with Jetphox, we present here two brief studies as an attempt to reduce the theoretical errors from the NLO calculation. These study the choice of renormalizaion and factorization scale parameter and secondly the jet algorithm parameters.

As studied in [480], the scale choice is set to a fraction of the photon $p_{T}$. By altering this fraction around the central value of 1.0 , it is hoped to gain an uncertainty on the terms missed in the NLO calculation. The best selection for this central value would be to be at a 'saddle point', where moving in any direction from this point gives similar changes in the cross section. However, it is found that as the scale is reduced (in steps: $2.0,1.0,0.5,0.25,0.1,0.05$ and 0.01 ) the cross section increases, when moving the two scales coherently or independantly. One difference in this result to the previous study was that it was carried out in three $p_{T}$ bins, but the result remained the same for all (only the highest bin was able to be calculated with a scale of 0.01 ). Similarly the addition of using Frixione isolation instead of the standard cone isolation also resulted in the same cross section behaviour. The summary of this is that there must be large contributions needed from NNLO. However, on the positive side, in all $3 p_{T}$ bins, the variation between 0.5-1.0-2.0 resulted in differences of similar magnitude around 1.0 , so this is likely a safe estimate of the uncertainty.

After the inclusive photon measurements, the next step experimentally is to require the addition of at least one jet. Using a jet of 10 GeV the cross section was calculated for two algorithms each for multiple sizes:

- Kt algorithm with $\Delta R=0.3,0.4,0.5$ or 0.6
- Cone with $\Delta R=0.4,0.5$ or 0.6

These choices had an affect of $<1 \%$ on the cross section computed in 3 photon $p_{T}$ bins, suggesting that this will not increase the error for the NLO calculation when moving from the inclusive cross section to that with an additional jet.

### 19.3 FRAGMENTATION PHOTONS IN PARTON-SHOWER MONTE-CARLO

The second part of this study continues to investigate photon isolation, but now in di-photon events using parton-shower Monte-Carlo generators; again the selection used is listed in the appendix. The study begins by investigating the distance between the photon and other particles. It then moves into studying several different styles of isolation criteria, including Frixione criteria as done in the inclusive NLO studies.
encodes the two photons in a symmetrized way.

### 19.31 Topology of fragmentation photons

We consider three sets of parton-shower Monte-Carlo samples for the $\gamma \gamma+\mathrm{X}$ process:

- Pythia [400] $\gamma \gamma$ Born and Box direct processes, plus the Pythia $\gamma+$ jet process with the jet fragmenting into a photon ( 20 million events were generated for the $\gamma+$ jet sample and 1000 times more would have been needed for the dijet fragmenting to two photons due to the low $q \rightarrow \gamma$ branching ratio for isolated photons).
- Pythia $\gamma \gamma$ Born and Box direct processes, plus the Pythia $\gamma+$ jet process with the jet fragmenting into a photon and the Pythia dijet process with the two jets fragmenting into photons. Both Pythia $\gamma+$ jet and dijet samples were generated with a filter which enhances the presence of events with isolated electromagnetic particles.
- Madgraph [165] $\gamma \gamma+$ up to two supplementary hard jets, with fragmentation/hadronization done with Pythia.
The fragmentation contribution is included as a bremsstrahlung contribution in Madgraph at matrix element level, while it is included as a showering contribution in Pythia $\gamma+$ jet and dijet (in the PYTHIA samples we identify fragmentation photons as those having a quark or gluor ${ }^{48}$ as parent). The fragmentation fraction found is compatible with ref [483]. We consider additionally the case where the two jets fragment into boosted neutral mesons ( $\pi^{0}, \eta, \rho$ and $\omega$ ) that can experimentally mimic direct or fragmentation photons at reconstructed level because of the finite granularity of the detector. These samples include an underlying event but were generated without pile-up.


Fig. 102: $\Delta R$ distance distribution between the photon and the other generator-level particle candidates in the event, for neutral mesons, fragmentation photons and partonic photons.

Fig. 102 shows the $\Delta R$ distance between the photon or neutral mesons and the other particle candidates in the event. Partonic photons, fragmentation photons and neutral mesons have different properties as a function of $\Delta R$. Partonic photons in Pythia have a linear behavior, which is expected because the only contribution that can enter in the isolation sum is the underlying event and pile-up (with also a small contribution from QCD radiation at the shower level) which is expected to be uniform in space. As each bin consists of an annulus with radius growing linearly as a function of $R$, the quantity

[^157]of particles grows linearly with $R$ in the area of the annulus. Neutral mesons have a radically different profile, with a peak of the $\Delta R$ distribution close to 0 . The peak is caused by the decay of particles resulting from jet fragmentation close to the neutral meson direction. Pythia fragmentation photons have a behavior somehow in between that of neutral mesons and partonic photons. The peak at low $\Delta R$ is still present but much reduced with respect to that of neutral mesons. Madgraph partonic photons exhibit a modulation of the Pythia partonic photon $\Delta R$ distribution, probably because Madgraph includes fragmentation as a bremsstrahlung contribution.

From this we can expect that the smaller the $\Delta R$ cone used in Frixione isolation (until $\Delta R \simeq 0.1$ ), the higher the discrimination against the neutral mesons and fragmentation photons. The discrimination against neutral mesons is higher than that against fragmentation photons (as is well-known experimentally). This can be seen in Fig. 103, which shows the isolation sum profile divided by the transverse energy of the photon for different cone sizes.


Fig. 103: Isolation sum normalized to the photon energy computed in cones of size $\Delta R<0.1$ (top left), $\Delta R<0.2$ (top right), $\Delta R<0.3$ (bottom left), $\Delta R<0.4$ (bottom right), for neutral mesons, fragmentation photons and partonic photons.

Table 14: Fraction represented by the 1-fragmentation and 2-fragmentation contributions for various Frixione isolation criteria in Pythia two-prompt photon samples (with electromagnetic enrichment filter).

| Criteria | 1-frag fraction | 2-frag fraction | 1,2-frag fraction |
| :---: | :---: | :---: | :---: |
| Solid $\Delta R<0.4, E_{T}^{\text {iso }}<5 \mathrm{GeV}$ | 0.335 | 0.157 | 0.492 |
| Hollow $0.1<\Delta R<0.4, E_{T}^{\text {iso }}<4 \mathrm{GeV}$ | 0.337 | 0.168 | 0.505 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=1.0$ | 0.322 | 0.145 | 0.467 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=0.2$ | 0.318 | 0.147 | 0.466 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.2$ | 0.372 | 0.228 | 0.599 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.1$ | 0.374 | 0.232 | 0.601 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=1.0$ | 0.353 | 0.192 | 0.545 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.5$ | 0.365 | 0.212 | 0.577 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.5, n=1.0$ | 0.343 | 0.176 | 0.518 |

### 19.32 Impact of hollow cones on the fragmentation contribution

In NLO generators, the products of the quark fragmentation are along the fragmentation photon direction. In parton-shower generators we have seen that this is not necessarily true. In NLO generators, the "hollow" or "crown" isolation, where the energy sum has to be below a fixed threshold in a region $R_{1}<\Delta R<R_{2}$ while in the region $R<R_{1}$ any arbitrary amount of energy is admitted, has been shown to enhance the fragmentation contribution with respect to the usual "solid" isolation. This "hollow" isolation is interesting also because this criterion is closer than the "solid" cone to what is used experimentally (it allows to exclude from the isolation sum the energy deposited by the photon itself). The first two lines of Tables 14 and 15 show that in general the fragmentation fraction does not increase significantly when moving from solid to hollow cone isolation, for the PYTHIA samples.

### 19.33 Impact of Frixione isolation on the fragmentation contribution

Tables 14 and 15 report the fragmentation fraction inside the Pythia two-prompt sample for different Frixione isolation criteria. Eight isolation cones were used : $\Delta R<0.05, \Delta R<0.1, \Delta R<0.15$, $\Delta R<0.2, \Delta R<0.25, \Delta R<0.3, \Delta R<0.35, \Delta R<0.4$. The results are almost identical if instead four cones are used ( $0.1,0.2,0.3,0.4$ ), as found at NLO. The tables show that in both the electromagnetically-enriched samples and non-enriched samples, the discrete Frixione isolation with the usual functional form $f(R)$ does not reduce the fragmentation contribution with respect to the standard isolation criterion (with a cone $\Delta R<0.4$ ) except when the parameter $\epsilon$ is at its smallest value, $\epsilon=$ 0.05 , for which modest reductions of between 5 and $8 \%$ can be achieved. The cause of this apparent non-optimal behavior can be explained by the non-collinearity of the fragmentation debris around the fragmentation photon in PYTHIA. Frixione isolation is designed to apply tighter and tighter isolation criteria $E_{T}^{i s o}<f(R) \rightarrow 0$ as $\Delta R \rightarrow 0$, assuming that most of the fragmentation debris are around $\Delta R \simeq 0$. As it is seemingly not the case in the parton-shower Monte-Carlo studied here, the criterion loses most of its discrimination power.

The previous study suggests that the previous working points studied with the Frixione functional form $f(R)$ might not be optimal for the rejection of fragmentation debris. In figure 104 we compare the performance of three different sets of criteria: 1) non-Frixione isolation in a single cone $\Delta R<0.4,2$ ) optimized working points for the parameters in the Frixione functional form (four cones $0.1,0.2,0.3,0.4$ were used to make the algorithm converge faster), 3) re-optimized 'Frixione' isolation criteria on cones $\Delta R<0.1,0.2,0.3,0.4$ without using the explicit functional form (we no longer constrain the events to satisfy $E_{T}^{i s o}<f(R)$ and let $f(R)$ free). In the second case, an optimization procedure is performed scanning over the parameters $\epsilon$ and $n$ to find the best working points (corresponding to a maximum

Table 15: Fraction represented by the 1 -fragmentation contribution for various Frixione isolation criteria in Pythia two-prompt photon samples (without enrichment filter).

| Criteria | 1-frag fraction |
| :---: | :---: |
| Solid $\Delta R<0.4, E_{T}^{i s o}<5 \mathrm{GeV}$ | 0.455 |
| Hollow $0.1<\Delta R<0.4, E_{T}^{i s o}<4 \mathrm{GeV}$ | 0.458 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=1.0$ | 0.420 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=0.2$ | 0.419 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.2$ | 0.514 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.1$ | 0.519 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=1.0$ | 0.489 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.5$ | 0.503 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.5, n=1.0$ | 0.465 |

efficiency for a given $s / b$ ). In the last case, an optimization code is used to find the best selection criteria to be applied on $E_{T}^{i s o}$ for each $\Delta R$ cone. The optimization takes as input the target value of $s / b$ (partonic signal over fragmentation background ratio), then relaxes and tightens each cut separately with an iterative procedure to find the best signal efficiency for this $s / b$ target. The procedure was performed to find the working points corresponding to the $s / b$ obtained with the first Frixione criterion.

Figure 104 shows that the optimized working points for the Frixione functional form perform slightly better than the standard isolation for a given photon efficiency, and that optimization using no functional form in turn performs slightly better than the Frixione functional form; for the same value of single-photon efficiency, lower values of fragmentation fraction are attainable. It should be noted that this optimisation leads to a looser cut on the first cone, $\Delta R<0.1$, than the usual functional form. Nevertheless, to obtain reductions in the fragmentation fraction of more than $10 \%$, increasingly significant reductions in single photon efficiency are required, since the fragmentation reduction becomes nearly flat.

All in all, with the definition of the isolation in a cone of $\Delta R$ used here, which is a usual way of defining isolation at the experimental level (where one has however to remove the footprint of the photon from the isolation sum and to cope with pile-up), rejecting fragmentation photons can be done only at a cost of a lowered signal efficiency. With this optimization procedure it was found that to decrease the fragmentation fraction by $10 \%$, a signal loss of about $60 \%$ has to be achieved, leading to extremely tight cuts probably not applicable in experimental analysis.

## CONCLUSIONS

Firstly for the NLO cross sections, it was found that only one of the Frixione isolation criteria suggested in [18] actually performs better at removing the fragmentation contribution in the inclusive case than that of the standard cone, although potentially too tight to use experimentally. However, it is useful to see that the results are independent of the number of cones used. This is also the case for the di-photon cross section where it compares well to the continuous criteria. A more promising result in the inclusive case is that the generalized version of Frixione isolation, with small values of $\epsilon$, do significantly reduce the fragmentation fraction without applying too tight a cut in the smallest cone. In addition it is confirmed that the 'saddle point' can not be found when altering the scale choice for the inclusive cross-section, suggesting more corrections needed at NNLO. Finally when moving to the photon with associated jet cross section, from the inclusive cross section, it is reported that the jet algorithm (or size) used at NLO makes little difference to the cross section.

In the study at the parton-shower level it was shown that the isolation profile of fragmentation


Fig. 104: The fraction of the 1 -fragmentation contribution vs single $\gamma$ efficiency for various sets of criteria. Blue : tested working points reported on table 15. Black : selection criteria on isolation in $\Delta R<0.4$. Green : Optimized Frixione isolation using the usual functional form. Red : Re-optimized isolation criteria on cones $\Delta R<0.1,0.2,0.3,0.4$ without using the functional form.
photons is no longer collinear anymore, whereas the modelization of the fragmentation function in NLO generators leads the quark/gluon debris to be collinear to the photon. Furthermore, the hadronization process of the quark/gluon that emitted the photon leads to a $\Delta R$ profile which is no longer peaked at zero (but close to zero). In parton-shower programs isolation still has increasing discriminating power when going lower in $\Delta R$. However, it was found that a $10 \%$ decrease in fragmentation fraction in diphoton events with respect to standard isolation leads to a drop in single photon signal efficiency to approximately $60 \%$ of the initial value. The usual functional form for Frixione isolation was shown to be not completely optimal for suppressing the fragmentation contribution while preserving high signal efficiency. This can be mitigated by re-optimizing the cuts for each $\Delta R$ of the discrete Frixione prescription, which allows a looser cut in the innermost cone. Further studies using other fragmentation modelizations in parton-shower programs like SHERPA [427] (LO matrix-element where photons and jets in the shower are matched to matrix element level) or POWHEG [484] (NLO matrix-element with consistent fragmentation photon matching) would need to be investigated.

In conclusion the results from the two studies show there are differences and similarities at the two levels. Regarding the fragmentation fraction, this is far more reduced at the NLO level than at the parton-shower level. However, the two levels show agreement that the results from Frixione isolation are independant of the number of cones used and that similar shape cuts can be obtained by retuning cuts at the parton-shower level and by using the generalized prescription at NLO.

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## APPENDIX: Selection details

All of the studies are carried out for $p p$ collisions at $\sqrt{S}=7 \mathrm{TeV}$. For simplicity the the inclusive studies are carried out for the region where the photon lies in $|\eta|<0.6$. When calculating the cone isolation around the photon a cone of 0.4 is used with the requirement that the energy in the cone is less than 4 GeV . The renormalization scale $\mu$ and initial state factorization scale $M$ are set to the photon $p_{T}$,
unless stated otherwise, and the CTEQ6.6 PDF[256] is used and the photon fragmentation functions are BFG set II [479]. For the generalized Frixione isolation case, the cones used are: $\mathrm{R}=0.4,0.35,0.3,0.25$, $0.2,0.15$ and 0.1.

In the NLO di-photon studies, the photons have: $p_{T}^{\gamma 1} \leq 25 \mathrm{GeV}, p_{T}^{\gamma 2} \geq 22 \mathrm{GeV}$, in the rapidity range $\left|\eta^{\gamma}\right| \leq 2.5$ for both photons, and a separation $\Delta R_{\gamma \gamma} \geq 0.4$ is required between the two photons. The mass range considered is $40 \mathrm{GeV} \leq m_{\gamma \gamma} \leq 300 \mathrm{GeV}$. In this case the scales $\mu$ and $M$ are chosen equal to $\min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}$.

In the parton shower di-photon studies, the photons are selected with: $M_{\gamma \gamma}>80 \mathrm{GeV}, p_{T}>21,20$ $\mathrm{GeV},|\eta|<2.5$ and $E_{T}^{i s o}<5 \mathrm{GeV}$.

## 20. EVENT-BY-EVENT PILEUP SUBTRACTION USING JET AREAS 49


#### Abstract

In these proceedings, we compare the efficiency of several jet-area-based subtraction methods to correct for pile-up contamination at hadronic colliders. We study the dependence on various variables like the $p_{t}$ and rapidity of the jets, the number of pile-up vertices or the Monte-Carlo generator variations. We conclude that estimations of the pile-up density using a median computed over grid-cell patches, including a rescaling to correct for the rapidity dependence, perform particularly well, though alternative methods are possible.


### 20.1 Introduction

With the LHC running at larger and larger luminosities, hard $p p$ interactions are accompanied by an increasing number of pile-up (PU) collisions: from a few PU events per bunch crossing in spring 2011, operation with $\sim 20 \mathrm{PU}$ events is now routine. Considering only in-time PU , this would lead to an extra transverse momentum of $\sim 750 \mathrm{GeV}$ deposited in the event, and a jet of a typical radius $R=0.5$ would see its transverse momentum shifted by $\sim 10 \mathrm{GeV}$. In order to obtain a good energy resolution for the jets it is therefore mandatory to correct for this contamination.

In these proceedings, we review several methods - both existing methods and new refinements - to subtract the contamination due to PU and provide a systematic study of their efficiency.

It is important to note already now that PU has not only the effect to shift the momentum of the jets: it also smears their momentum. Indeed, the number of PU vertices varies from one collision to the next (following a Poisson distribution varying with the beam conditions), all PU interactions, i.e. minimum bias collisions, do not lead to the same energy deposit, and finally, the energy produced in a minimum bias collision is not deposited uniformly across the detector. Altogether, on top of an average shift, PU will add two sources of resolution smearing: event-to-event and in-event fluctuations corresponding respectively to variations of the PU activity from one event to another and from one point to another in a single event.

Here we shall primarily study in-time $P U$, that is the effects coming from multiple $p p$ interactions that occur in the same bunch crossing as the hard interaction one triggers on. Because of the response time inherent to each detector this would come with a second effect, out-of-time $P U$, corresponding to the PU activity in the few bunch crossings preceding the one with the hard interaction. Since these heavily depend on the details of each individual detector - and even varies from one sub-detector to another - it goes beyond the scope of this theoretical study. However, as we shall discuss in further detail later on, the PU subtraction methods proposed here do not make any assumption about a distinction between in-time and out-of-time PU and thus should be robust enough in more complex cases.

[^158]
### 20.2 Subtraction method(s)

We are interested in the situation where a hard event is contaminated by a background coming from additional pileup interactions. A reconstructed jet in that full event (hard event + background), which we shall call a full jet, differs from the hard jet in the original hard event because of the presence of the background. By background subtraction, we mean correcting the full jet in such as to recover the momentum of the original hard jet, i.e. subtract the pileup contamination from the jet's momentum.

### 20.21 Background effects

Our starting point is to realise [485] that a uniform background affects the momentum of a jet in two ways: it shifts its momentum because of the background particles clustered with the jet, and it modifies the way the hard particles themselves are clustered because the background particles are not infinitely soft.

This means that the reconstructed momentum has the form 50

$$
\begin{equation*}
p_{t, \text { full }}=p_{t, \text { hard }}+\rho A \pm \sigma \sqrt{A}+\Delta p_{t}^{B R} \tag{20.2.1}
\end{equation*}
$$

where $p_{t}$ denotes the transverse momentum of the reconstructed jet, $p_{t, \text { hard }}$ the momentum of the original hard jet (in the absence of PU), $A$ the jet area, $\rho$ the background density per unit area within a given event, $\sigma$ the fluctuations of that background (per unit area) from place to place within the event, and $\Delta p_{t}^{B R}$ the back-reaction describing the effect of the background particles on the clustering of the hard ones.

If the background has a positional dependence (e.g. depends on rapidity) then $\rho$ and $\sigma$ will depend on the position of the jet one tries to subtract.

Eq. 20.2.1) characterises the fact that the background has the effects of shifting the transverse momentum of the jet and to degrade its resolution. The shift comes from the " $\rho$ " term in 20.2.1) and from potential back-reaction systematic effects. Using the anti- $k_{t}$ jet algorithm the shift due to backreaction is negligibl ${ }^{51}$. Resolution smearing effects come from various sources: the fluctuations of the background from within an event, i.e. the " $\sigma$ " term in 20.2.1, fluctuations of the background from one event to another, that is the fact that $\rho$ is not the same in every event, and the fluctuations in the back-reaction.

### 20.22 Central subtraction formula

From (20.2.1], the natural way to subtract the background contamination is to define the subtracted jet as [485]

$$
\begin{equation*}
p_{t, \text { sub }}=p_{t}-\rho_{\mathrm{est}} A \tag{20.2.2}
\end{equation*}
$$

where $\rho_{\text {est }}$ is the estimated value for the background density per unit area.
To apply this subtraction we need to compute the jet area and find an estimation $\rho_{\text {est }}$ for the background density per unit area. The jet areas are readily available using FastJet, so we just need to focus on $\rho_{\text {est }}$. The main goal of these proceedings is to investigate various methods of obtaining $\rho_{\text {est }}$ which are listed below. In all cases, it is primordial to realise that the determination of $\rho_{\text {est }}$ is performed event-by-event, and even jet-by-jet when the positional dependence of the background is taken into account.

As we shall see later on, the fact that $\rho$ is estimated for each individual event is crucial: it corrects for the fluctuations of the background from one event to another. If instead one uses an averaged value for $\rho_{\text {est }}$ (over many events), one would get an extra resolution smearing due to the fluctuations of $\rho$ across different events. Similarly, the jet area $A$ in 20.2.2) has to be computed for each individual jet. Using an average area would lead to an additional source of fluctuations of the form $\rho \sqrt{\left\langle A^{2}\right\rangle-\langle A\rangle^{2}}$.

[^159]Using seen vertices Since experimentally it might be possible - within some level of accuracy that goes beyond the scope of this discussion - to count the number of pileup vertices using charged track reconstruction, one appealing way to estimate the background density in a given event would be to count these vertices and subtract a pre-determined number for each of them:

$$
\begin{equation*}
\rho_{\mathrm{est}}^{(n \mathrm{PU})}(y)=f(y) n_{\mathrm{PU}, \text { seen }}, \tag{20.2.3}
\end{equation*}
$$

where we have made explicit the fact that the proportionality constant $f(y)$ can carry a rapidity dependence. $f(y)$ can be studied from minimum bias collisions (see Section 20.32 below) and can take into account the fact that only a fraction of the PU vertices will be reconstructed.

Median subtraction This technique divides the rapidity-azimuthal angle plane in patches and estimates $\rho$ for each event using

$$
\begin{equation*}
\rho_{\text {est }}^{(\text {global })}=\operatorname{median}_{i \in \text { patches }}\left\{\frac{p_{t, i}}{A_{i}}\right\} \tag{20.2.4}
\end{equation*}
$$

This is motivated by the observation that many regions in the event are populated just by the background. In these regions, $p_{t} / A$ is an estimate of $\rho$ and the use of the median, rather than the average, which ensures reduced bias from the hard jets.

This method was originally proposed in [485] using jets (from a $k_{t}$ or Cambridge/Aachen clustering) as patches. Here, we shall also test a new option where the $y-\phi$ plane is simply subdivided into grid cells that we use as patches.

Using a local range Eq. 20.2.4 provides a unique, global, estimate of $\rho$ for the event but does not take into account the positional-dependence of the background. One option, assuming one wants to estimate $\rho$ at the location of a jet $j$, is to limit the computation of the median to the jets in the vicinity of $j$, that i. 5

$$
\begin{equation*}
\rho_{\text {est }}^{(\text {local })}(j)=\underset{\text { jets } i \in \mathcal{R}(j)}{\operatorname{median}}\left\{\frac{p_{t, i}}{A_{i}}\right\} \tag{20.2.5}
\end{equation*}
$$

where $\mathcal{R}(j)$ is a local range around $j$. A typical example, that we shall study later on, is the case of a strip range where only the jets with $\left|y-y_{j}\right|<\Delta$ are included. This option was already proven to be powerful in [486].

Using rescaling Another option to correct for the rapidity dependence of the background ${ }^{53}$ is to introduce a pre-computed rapidity-reshaping function $f(y)$ (see Section 20.32) and use

$$
\begin{equation*}
\rho_{\text {est }}^{(\text {resc. })}(y)=f(y) \operatorname{median}_{i \in \text { patches }}\left\{\frac{p_{t, i}}{A_{i} f\left(y_{i}\right)}\right\} \tag{20.2.6}
\end{equation*}
$$

where now all patches (jets or grid cells) are included in the computation of the median.

### 20.3 Performance tests

### 20.31 Testing framework

The remainder of these proceedings will be devoted to an in-depth comparison of the subtraction methods proposed in Section 20.2. Our testing framework will be very similar to the one used in [486]: we embed a hard event into a pileup background (see again Section 20.2, we reconstruct and subtract the jets in

[^160]both the hard and full event $s^{54}$. for each jet in the hard event, we find the matching jet in the full event and compute the shift
\[

$$
\begin{equation*}
\Delta p_{t}=p_{t}^{\mathrm{full}, \mathrm{sub}}-p_{t}^{\mathrm{hard}, \mathrm{sub}}, \tag{20.3.1}
\end{equation*}
$$

\]

i.e. the difference between the reconstructed-and-subtracted jet with and without pileup. A positive (resp. negative) $\Delta p_{t}$ would mean that the PU contamination has been underestimated (resp. overestimated).

Though in principle there is some genuine information in the complete $\Delta p_{t}$ distribution - e.g. it could be useful to deconvolute the extra smearing brought by the pileup, see e.g. [486] and [487] - we shall focus on two simpler quantities: the average shift $\left\langle\Delta p_{t}\right\rangle$ and the dispersion $\sigma_{\Delta p_{t}}$. While the first one is a direct measure of how well one succeeds at subtracting the pileup contamination on average, the second quantifies the remaining effects on the resolution. One thus wishes to have $\left\langle\Delta p_{t}\right\rangle$ close to 0 and $\sigma_{\Delta p_{t}}$ as small as possible. Note that these two quantities can be studied as a function of variables like the rapidity and transverse momentum of the jets or the number of pileup interactions. In all cases, a flat behaviour would indicate a robust subtraction method.

The robustness of our conclusions can be checked by varying many ingredients:

- one can study various hard processes with the hope that the PU subtraction is not biased by the hard event. In what follows we shall study dijets with $p_{t}$ ranging from 50 GeV to 1 TeV , as well as fully hadronic $t \bar{t}$ events as a representative of busier final states.
- The Monte-Carlo used to generate the hard event and PU can be varied. For the hard event, we have used Pythia 6.4.24 [400] with the Perugia 2011 tune, Pythia 8.150 with tune 4C [348] and Herwig 6.5.10 [488] with the ATLAS tune and we have switched multiple interactions on (our default) or off. For the minimum bias sample used to generate PU, we have used Pythia 8, tune 4C, and checked that our conclusions remain unchanged when using Herwig++ [489] (tune LHC-UE7-2).

Additional details of the analysis For the sake of completeness, we list here the many other details of how the $\Delta p_{t}$ analysis has been conducted: we have considered particles with $|y| \leq 5$ with no $p_{t}$ cut or detector effect; jets have been reconstructed with the anti- $k_{t}$ algorithm with $R=0.5$ keeping jets with $|y| \leq 4$; for area computations, we have used active areas with explicit ghosts with ghosts placed ${ }^{55}$ up to $|y|=5$; for jet-based background estimations, we have used the $k_{t}$ algorithm with $R=0.4$ though other options will be discussed (and the 2 hardest jets in the set have been excluded from the median computation to reduce the bias from the hard event); for grid-based estimations the grid extends up to $|y|=5$ with cells of edge-size 0.56 (other sizes will be investigated); for estimations using a local range, a strip range of half-width 1.5 has been used and we refer to the Section 20.32 below for more information about the rapidity rescaling. Jet reconstruction, area computation and background estimation have all been carried out using FastJet (v3) [361, 435]. Pile-up is generated as a superposition of a Poissondistributed number of minimum bias events and we will vary the average number of pileup interactions. We shall always assume $p p$ collisions with $\sqrt{s}=7 \mathrm{TeV}$. Finally, the matching of a full jet to a hard jet is made by requiring that their common constituents contribute for at least $50 \%$ of the transverse momentum of the hard jet. We shall not discuss matching efficiencies here but they are extremely good: for a reconstructed (full) jet of 50 GeV and 20 PU events, the matching efficiency is $99.9 \%$ and this increases to $99.98 \%$ for $p_{t} \geq 50 \mathrm{GeV}$ and 5 PU events and $99.995 \%$ for $p_{t} \geq 100 \mathrm{GeV}$ and 20 PU events.

### 20.32 Minimum bias and rapidity shape

Before discussing the performances of the subtraction methods described in Section 20.2, there is still a building block that has to be discussed, namely the rapidity dependence of the background $f(y)$ that

[^161]

Fig. 105: Rapidity dependence of the transverse energy per unit area deposited in minimum bias events (obtained from Pythia 8, tune 4C). The normalisation of the fit is such that $f_{\text {seen }}$ is the fraction of seen minimum bias events i.e. the fraction of events which have at least 2 charged tracks with $|y| \leq 2.5$ and $p_{t} \geq 100 \mathrm{MeV}$.
enters in Eqs. 20.2.3) and 20.2.6). Letting aside the question of in-time vs. out-of-time PU and nonlinear effects in the detectors, the shape $f(y)$ can be obtained directly from minimum bias events.

In our case, we have generated minimum bias events with Pythia 8 (tune 4C) and studied the rapidity dependence of the transverse momentum deposited per unit area. The result is shown on Fig. 105 together with a quartic fit. If $f(y)$ is used to rescale median-based estimates of $\rho$, Eq. 20.2.6, any global normalisation factor would cancel, but in the case of Eq. 20.2.3) i.e. for the "seen vertices" method, the normalisation has to match what we mean by a seen PU vertex. In what follows, we shall define that as a minimum bias interaction that has at least 2 charged tracks with $|y| \leq 2.5$ and $p_{t} \geq 100$ MeV , which corresponds to $69.7 \%$ of the event ${ }^{56}$. In these conditions, we have found that the rapidity dependence is well reproduced by

$$
\begin{equation*}
f(y)=1.051141-0.023608 y^{2}+0.000026 y^{4} . \tag{20.3.2}
\end{equation*}
$$

### 20.33 Generic performance and rapidity dependence

Let us begin our performance benchmarks by the study of the rapidity dependence of PU subtraction. First of all, Fig. 106 shows the residual average shift $\left(\left\langle\Delta p_{t}\right\rangle\right)$ as a function of the rapidity of the hard jet. These results are presented for different hard processes, generated with Pythia 8 and assuming an average of 10 PU events per hard interaction. Robustness w.r.t. that choice will be discussed in the next Section but does not play any significant role for the moment.

The first observation is that the subtraction based on the number of seen PU vertices does a very good job in all 3 cases. Then, global median-based (using jets or grid cells) estimations of $\rho$, i.e. the (red) square symbols, do a fair job on average but, as expected, fail to correct for the rapidity dependence of the PU contamination. If one now restricts the median to a rapidity strip around the jet, the (blue) triangles, or if one uses rapidity rescaling, the (black) circles, the residual shift is very close to 0 , typically a few hundreds of MeV , and flat in rapidity.

Note that the strip-range approach seems to have a small residual rapidity dependence and overall offset for high- $p_{t}$ processes or multi-jet situations. That last point, more clearly observed with some

[^162]

Fig. 106: Residual average shift as a function of the jet rapidity for all the considered subtraction methods. For the left (resp. centre, right) plot, the hard event sample consists of dijets with $p_{t} \geq 50 \mathrm{GeV}$ (resp. dijets with $p_{t} \geq 400 \mathrm{GeV}$, and jets above $p_{t} \geq 50 \mathrm{GeV}$ in $t \bar{t}$ events), generated with Pythia 8 (tune 4 C ) in all cases. The typical PU contamination (for unsubtracted jets) is around 5 GeV .

Monte-Carlo generators like Pythia 6 than with others, may be due to the fact that smaller ranges tend to be more affected by the presence of the hard jets (see e.g. Appendix A. 2 of [486]), an effect which is reinforced for multi-jet events. The fact that the residual shift seems a bit smaller for grid-based estimates will be discussed more extensively in the next Section.

Next, we turn to the dispersion of $\Delta p_{t}$, a direct measure of the impact of PU fluctuations on the $p_{t}$ resolution of the jets. Our results are plotted in Fig. 107 as a function of the rapidity of the hard jet (left panel), the number of PU vertices (central panel) and the transverse momentum of the hard jet (right panel). All subtraction methods have been included as well as the dispersion one would observe if no subtraction were performed.

The results show a clear trend: first, a subtraction based on the number of seen PU vertices bring an improvement compared to not doing any subtraction; second, median-based estimations of $\rho$ give a more significant improvement; and third, all median-based approaches perform similarly well.

The reason why median-based estimations of $\rho$ outperform the estimation based on the number of seen PU vertices is simply because minimum bias events do not all yield the same energy deposit and this leads to an additional source of fluctuations in the "seen vertices" estimation compared to all median-based ones. This is the main motivation for using an event-by-event determination of $\rho$ based on the energy deposited in the event. This motivation is further strengthened by the fact that additional issues like vertex resolution or out-of-time PU would affect both $\left\langle\Delta p_{t}\right\rangle$ and $\sigma_{\Delta p_{t}}$ if estimated simply from the number of seen vertices while median-based approaches are more robust.

Note finally that even though local ranges and rapidity rescaling do correct for the rapidity dependence of the PU on average, the dispersion still depends on rapidity. The increase with the number of PU vertices is in agreement with the expected $\sqrt{n_{\mathrm{PU}}}$ behaviour and the increase with the $p_{t}$ of the hard process can be associated with back-reaction, see [486]. These numbers can also be compared to the typical detector resolutions which would be $\sim 10 \mathrm{GeV}$ for 100 GeV jets and $\sim 20 \mathrm{GeV}$ at $p_{t}=400 \mathrm{GeV}$ [490, 491].

### 20.34 Robustness and Monte-Carlo dependence

The last series of results we want to present addresses the stability and robustness of the median-based estimation of the PU density per unit area.

To do that, the first thing we shall discuss is the Monte-Carlo dependence of our results. In Fig.


Fig. 107: Dispersion $\sigma_{\Delta p_{t}}$. Each curve corresponds to a different subtraction method and the results are presented as a function of different kinematic variables: left, as a function of the rapidity of the hard jet for a sample of jets with $p_{t} \geq 100 \mathrm{GeV}$ and assuming an average of 10 PU events; centre: as a function of the number of PU events for a sample of jets with $p_{t} \geq 100$; right: as a function of the $p_{t}$ of the hard jet, assuming an average of 10 PU events


Fig. 108: Dependence of the average $p_{t}$ shift as a function of the number of PU vertices for various Monte-Carlo generators. For the left plot, the hard sample is made of dijets with $p_{t} \geq 100 \mathrm{GeV}$ while for the right plot, we have used a hadronic $t \bar{t}$ sample. For each generator, we have considered both the case with the Underlying Event switched on (filled symbols) and off (open symbols). All results have been obtained using a grid-based median estimation of $\rho$ using rapidity rescaling.


Fig. 109: Average residual shift after PU subtraction. $\left\langle\Delta p_{t}\right\rangle$ is plotted as a function of the $p_{t}$ of the jet for an average of 10 PU events (left panel), or as a function of the number of PU vertices for dijets with $p_{t} \geq 100 \mathrm{GeV}$ (central panel) and for $t \bar{t}$ events (right panel). In all cases, we compare 3 methods: the rapidity-strip range, (red) triangles, the jet-based approach with $y$-rescaling, (blue) circles, and the gridbased approach with $y$ rescaling, (black) squares. Each curve is the result of averaging over the various Monte-Carlo generator options and the dispersion between them is represented both as error bars on the top row and directly on the bottom row.

108 we compare the different Monte-Carlo predictions for the $\left\langle\Delta p_{t}\right\rangle$ dependence on the number of PU vertices in the case of a grid-based median estimate of $\rho$ with rapidity rescaling. For each of the three considered Monte-Carlos, we have repeated the analysis with and without Underlying Event (UE) in the hard event. The first observation is that all the results span a range of $300-400 \mathrm{MeV}$ in $\Delta p_{t}$ and have a similar dependence on the number of PU vertices. The dependence on $n_{\mathrm{PU}}$ is flat for dijet events but shows a small decrease for the busier $t \bar{t}$ events. The $300-400 \mathrm{MeV}$ shift splits into a $100-200 \mathrm{MeV}$ effect when changing the generator, which is likely due to the small but non-zero effect of the hard event on the median computation, and a $100-200 \mathrm{MeV}$ effect coming from the switching on/off of the UE.

This question of subtracting the UE deserves a discussion: since the UE is also a soft background which is relatively uniform, it contributes to the median estimate and, therefore, one expects the UE, or at least a part of it, to be subtracted together with the PU. Precisely for that reason, when we compute $\Delta p_{t}$, our subtraction procedure is not applied only on the "full jet" (hard jet+PU) but also on the hard jet, see Eq. 20.3.1. The $100-200 \mathrm{MeV}$ negative shift observed in Fig. 108 thus means that, when switching on the UE, one subtracts a bit more of the UE in the full event (with PU) than in the hard event alone (without PU). This could be due to the fact (see [492] for details) that for sparse events, as is typically the case with UE but no PU, the median tends to slightly underestimate the "real" $\rho$, e.g. if half of the event is empty, the median estimate would be 0 . This is in agreement with the fact that for $t \bar{t}$ events, where the hard event is busier, switching on the UE tends to have a smaller effect. Note finally that as far as the size of the effect is concerned, this $100-200 \mathrm{GeV}$ shift has to be compared with the $\sim 1 \mathrm{GeV}$ contamination of the UE in the hard jets.

Finally, we wish to compare the robustness of our various subtraction methods for various processes i.e. hard events and PU conditions. In order to avoid multiplying the number of plots, we shall treat the Monte-Carlo (including the switching on/off of the UE) as an error estimate. That is, an average measure and an uncertainty will be extracted by taking the average and dispersion of the 6 Monte-Carlo setups. The results of this combination are presented on Fig. 109 for various situations and subtraction


Fig. 110: Left: relative difference between the reconstructed jet and the reconstructed $Z$ boson transverse momenta. Right: at a given $p_{t}$ of the reconstructed $Z$ boson, difference between the reconstructed $p_{t}$ of the jet and the ideal $p_{t}$ with no UE or PU, i.e. $p_{t}$ shift w.r.t. the "noUE" curve, the (black) triangles, on the left panel. See the text for the details of the analysis.
methods. For example, the 6 curves from the left plot of Fig. 108 have been combined into the (black) squares of the central panel in Fig. 109 .

Two pieces of information can be extracted from these results. First of all, for dijets, the quality of PU subtraction is, to a large extent, flat as a function of the $p_{t}$ of the jets and the number of PU vertices. When moving to multi-jet situations, we observe an additional residual shift in the $100-300 \mathrm{MeV}$ range, extending to $\sim 500 \mathrm{MeV}$ for the rapidity-strip-range method. This slightly increased sensitivity of the rapidity-strip-range method also depends on the Monte-Carlo. While in all other cases, our estimates vary by $\sim 100 \mathrm{MeV}$ when changing the details of the generator, for multi-jet events and the rapidity-strip-range approach this is increased to $\sim 200 \mathrm{MeV}$.

Overall, the quality of the subtraction is globally very good. Methods involving rapidity rescaling tends to perform a bit better than the estimate using a rapidity strip range, mainly a consequence of the latter's greater sensitivity to multi-jet events. In comparing grid-based to jet-based estimations of $\rho$, one sees that the former gives slightly better results, though the differences remain small.

Since the grid-based approach is considerably faster than the jet-based one, as it does not require an additional clustering of the even ${ }^{57}$, the estimation of $\rho$ using a grid-based median with rapidity rescaling comes out as a very good default for PU subtraction. One should however keep in mind local-range approaches for the case where the rapidity rescaling function cannot easily be obtained.

### 20.4 PU v. UE subtraction: an analysis on $Z+j e t$ events

To give further insight on the question of what fraction of the Underlying Event gets subtracted together with the pileup, we have performed an additional study of $Z+$ jet events. We look at events where the $Z$ boson decays into a pair of muons. We have considered 5 different situations: events without PU or UE, events with UE but no PU subtracted or not, and events with both UE and PU again subtracted or not. Except for the study of events without UE, this analysis could also be carried out directly on data.

Practically, we impose that both muons have a transverse momentum of at least 20 GeV and have $|y| \leq 2.5$, and we require that their reconstructed invariant mass is within 10 GeV of the nominal $Z$

[^163]mass. As previously, jets are reconstructed using the anti- $k_{t}$ jet algorithm and the pileup subtraction is performed using the grid-based-median approach with rapidity rescaling and a grid size of 0.55 . All events have been generated with Pythia 8 (tune 4C) and we have assumed an average PU multiplicity of 20 events.

In Fig. 110, we have plotted the ratio $p_{t, \text { jet }} / p_{t, Z}-1$, with $p_{t, \text { jet }}$ the transverse momentum of the leading jet, for the various situations under considerations. Compared to the ideal situation with no PU and no UE, the (black) triangles, one clearly sees the expected effect of switching on the UE, the empty (green) circles, or adding PU, the empty (red) squares: the UE and PU add to the jet $\sim 1.2$ and 13 GeV respectively.

We now turn to the cases where the soft background is subtracted, i.e. the filled (blue) squares and (magenta) circles, for the cases with and without PU respectively. There are two main observations:

- with or without PU, the UE is never fully subtracted: from the original $1-1.5 \mathrm{GeV}$ shift, we do subtract about 800 MeV to be left with a $0-500 \mathrm{MeV}$ effect from the UE. That effect becomes smaller and smaller when going to large $p_{t}$.
- in the presence of PU, the subtraction produces results very close to the corresponding results without PU and where only the UE is subtracted. This nearly perfect agreement at large $p_{t, \text { jet }}$ slightly degrades into an additional offset of a few hundreds of MeV when going to smaller scales. This comes about for the following reason: the non-zero $p_{t}$ resolution induced by pileup (even after subtraction) means that in events in which the two hardest jets have similar $p_{t}$, the one that is hardest in the event with pileup may not correspond to the one that is hardest in the event without pileup. This introduces a positive bias on the hardest jet $p_{t}$ (a similar bias would be present in real data even without pileup, simply due to detector resolution). The "matched" curve in Fig. 110 (right) shows that if, in a given hard event supplemented with pileup, we explicitly use the jet that is closest to the hardest jet in that same event without pileup, then the offset disappears, confirming its origin as due to resolution-related jet mismatching.


### 20.5 Conclusions and discussion

In these proceedings, we have investigated several methods to correct for the pile-up contamination to jets. They are all based on the observation that the average PU contribution to a jet is on average proportional to its area, which directly leads to eq. 20.2.2. The various methods then differ by the method used to estimate the PU activity per unit area, $\rho$. The subtraction efficiency has been studied by embedding hard events into PU backgrounds and investigating how jet reconstruction was affected by measuring the remaining $p_{t}$ shift after subtraction $\left(\left\langle\Delta p_{t}\right\rangle\right)$ as well as the impact on resolution ( $\sigma_{\Delta p_{t}}$ ).

There are 3 broad approaches to the estimation of $\rho$ : (a) using an average contamination per PU vertex, the seen vertices approach, (b) using an event-by-event estimation and, the median approach with jets or grid cells as patches, and (c) using an event-by-event and jet-by-jet method, the local range or rescaling approaches.

The first important message is that, though all methods give a very good overall subtraction $\left(\left\langle\Delta p_{t}\right\rangle \approx 0\right.$ ), event-by-event methods should be preferred because their smaller PU impact on the $p_{t}$ resolution (see Fig. 107). This is mostly because the "seen vertices" method has an additional smearing coming from the fluctuations between different minimum bias collisions. This does not happen in event-by event methods that are only affected by point-to-point fluctuations in an event. Note also that event-by-event methods are very likely more robust than methods based on identifying secondary vertices when effects like vertex identification and out-of-time PU are taken into account.

The next observation is that event-by-event and jet-by-jet methods have the additional advantage that they correct for positional-dependence of the background like its rapidity dependence (see Fig. 106). The median approach using a local range (with jets as patches) or rapidity rescaling (using jets or grid cells as patches) all give an average offset in the $0-300 \mathrm{MeV}$ range, independently of the rapidity of
the jet, its $p_{t}$ or the number of PU vertices, see Fig. 109 and are thus very suitable methods for PU subtraction at the LHC. Pushing the analysis a bit further one may argue that the local-range method has a slightly larger offset when applied to situations with large jet multiplicity like $t \bar{t}$ events (the right panel of Fig. (109) though this argument seems to depend on the Monte-Carlo used to generate the hard-event sample. Also, since it avoids clustering the event a second time, the grid-based method has the advantage of being faster than the jet-based approach.

At the end of the day, we can recommend the median-based subtraction method with rapidity rescaling and using grid cells as patches as a powerful default PU subtraction method at the LHC. But one should keep in mind that the use of jets instead of grid cells also does a very good job and that local-ranges can be a good alternative to rapidity rescaling if the rescaling function cannot be computed. Also, though we have not discussed that in detail, a grid cell size of 0.55 is a good default as is the use of $k_{t}$ jets with $R=0.4$.

To conclude, let us make a few general remarks. First, our suggested method involves relatively few assumptions, which helps ensure its robustness. Effects like in-time v. out-of-time PU or detector response should not have a big impact. Many of the studies performed here can be repeated with "real data" rather than Monte-Carlo simulations. The best example is certainly the $Z+$ jet study of Section 20.4 which could be done using data samples with different PU activity from 2010 and 2011. Also, the rapidity rescaling function can likely be obtained from minimum bias collision data and the embedding of a hard event into pure PU events could help quantifying the remaining $\mathcal{O}(100 \mathrm{MeV})$ bias. Experimentally, it would also be interesting to investigate hybrid techniques where one would discard the charged tracks that do not point to the primary vertex and apply the subtraction technique described here to the rest of the event. This would have the advantage to further reduce fluctuation effects (roughly by a factor $\sim \sqrt{1 /\left(1-f_{\mathrm{chg}}\right)} \approx 1.6$, where $f_{\mathrm{chg}} \approx 0.61$ is the fraction of charged particles in an event). Finally, all the facilities to compute jet areas and background estimation - including jets or grid-cells as patches, local ranges and rescaling functions - are readily available from FastJet (v3.0.0 onward) using e.g. the GridMedianBackgroundEstimator or Subtractor tools.

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## Part VI

## MC TUNING AND OUTPUT FORMATS

## 21. TUNE KILLING: QUANTITATIVE COMPARISONS OF MC GENERATORS AND TUNES ${ }^{58}$


#### Abstract

We summarise the implementation, status, and scope of the "tune killing" project, which classifies MC generator codes and tunes according to their quality of data description across a range of LHC-relevant observables. The primary aim of the project is to provide sufficiently clear information about generator performance that the current large collection of available tunes may be objectively reduced to a more manageable standard set for common use by LHC experiments and phenomenologists. We make final recommendations as


[^164]to which generators and tunes are in rude health, and those which are obvious candidates for retirement from active service.

### 21.1 INTRODUCTION

Popular MC generators are nowadays associated with a bewildering array of standard parameter configurations, called "tunes". This proliferation of tunes is due to the ongoing project to provide optimised descriptions of LEP, Tevatron and LHC data: as new data and techniques have become available, new tunes have been created, usually but not always with increasing quality of data description. This process looks set to continue, and hence there is a need for agreement on which tunes are of most common interest at a given time.
The PYTHIA6 [400] event generator in particular has been the de facto testbed for tuning due to the wealth of community expertise and its ubiquity of tuning parameters for physical processes. At the time of writing there are 77 tunes available via the built-in PYTUNE routine, and a further 10 or more presented by the ATLAS experiment alone (this counting of ATLAS tunes includes equivalently weighted tunes for multiple PDFs, but not systematic variation tunes, of which there are many more). With such a profligacy of configuration options, it is difficult to objectively decide which are to be preferred for LHC simulation without manually cross-referencing hundreds of plots. It is hence not uncommon for different experimental or phenomenological studies to use entirely disjoint MC generator setups, making comparison difficult. Ideally we would have a much smaller set of agreed-upon generator setups, but choosing such a privileged subset requires clear information on which to base our preferences.
As a first step to addressing this issue, we present here a comparative study of event generator codes and tunes across a range of observables, particularly those of relevance for LHC physics. The study is based on analyses from the Rivet [360] toolkit, and the resulting data descriptions are quantitatively scored based on measures of deviation from the data values, including $\chi^{2}$ and median/maximum binwise deviations (in units of combined experimental, statistical, and theoretical uncertainties). The results are presented as a series of Web pages, using colour coded tables which are hyperlinked to provide the necessary information in a compact, hierarchical form.

### 21.2 Analysis system

The data analysed for this project was produced by individual runs of various generator/tune configurations into the Rivet analysis system. A choice of Rivet analyses was made, intended to cover a number of core QCD modelling aspects for LHC physics: these are documented in Table 16. In some cases only the most relevant range in the distribution is included, as indicated in the Table. The generators and tunes used are documented in Table 17
Note that not all observables are suitable for all generators. For example, AlpGen has not been used for LEP fragmentation, although in a future iteration we will extend the AlpGen coverage to include underlying event observables, where the hard jets could interfere with those from the multiple parton interaction (MPI) mechanism. Several observables, notably hard photon physics, minimum bias observables, and fragmentation/strangeness from RHIC and LHC have not yet been included: this is envisaged as a future extension of the project.
A Python program was written to load the histogram files for each generator/tune combination from a hierarchical directory structure, and to perform some basic statistical characterisation on each bin, histogram, and semantic group of histograms. At the histogram level, specifications are used to determine which bins are to be considered in the statistical comparisons, and to add a nominal "theoretical uncertainty". In this study a $10 \%$ theoretical uncertainty was added to the underlying event and fragmentation observables and a $5 \%$ theoretical uncertainty on the rest. The combined uncertainty for each bin $b$ is then computed from the sum in quadrature of the reference data error, the MC statistical error and the theoretical uncertainty, and is used to compute a MC-data deviation for that bin, expressed in units of

| Observable | Rivet analysis | Ref. | Range |
| :---: | :---: | :---: | :---: |
| Underlying event |  |  |  |
| Transverse region $N_{\text {ch }}$ vs. $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Transverse region $\sum p_{\perp}$ vs. $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Transverse region $\left\langle p_{\perp}\right\rangle$ vs $N_{\text {ch }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] |  |
| Jets |  |  |  |
| Toward region $N_{\text {ch }}$ vs $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Toward region $\sum p_{\perp}$ vs $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Jet shapes, $30<p_{\perp}<40 \mathrm{GeV}$, $\|y\|<2.8$ | ATLAS_2011_S8924791 | [494] |  |
| Jet shapes, $310<p_{\perp}<400 \mathrm{GeV},\|y\|<2.8$ | ATLAS_2011_S8924791 | [494] |  |
| Dijet $\Delta \phi, 110<p_{\perp}<160 \mathrm{GeV}$ | ATLAS_2011_S8971293 | [495] | $3 \pi / 4 \rightarrow \pi$ |
| Dijet $\Delta \phi, 310<p_{\perp}<400 \mathrm{GeV}$ | ATLAS_2011_S8971293 | [495] | $3 \pi / 4 \rightarrow \pi$ |
| Dijet mass, $0.3<\|y\|<0.8$, anti- $k_{\perp}(0.4)$ | ATLAS_2010_S8817804 | [382] |  |
| Transverse thrust, $90 \mathrm{GeV}<p_{\perp}^{\text {jet1 }}<125 \mathrm{GeV}$ | CMS_2011_S8957746 | [496] |  |
| ISR/intrinsic- $k_{\perp}$ |  |  |  |
| DØ $\phi^{*},\|y\|<1.0$ | D0_2010_S8821313 | [497] | $\phi^{*}<0.4$ |
| DØ $\phi^{*}, 1.0<\|y\|<2.0$ | D0_2010_S8821313 | [497] | $\phi^{*}<0.4$ |
| Fragmentation |  |  |  |
| $N_{\text {ch }}, \pi^{+} / \pi^{-}, K^{+} / K^{-}$at LEP | DELPHI_1996_S3430090 | [498] |  |
| $\rho / \pi, K / \pi, \Sigma^{ \pm,+,-, 0} / \pi, p / \pi, \Lambda / \pi$ | PDG_HADRON_MULTIPLICITIES | [499] |  |
| Inclusive $x_{p}$, thrust (+ major \& minor) | DELPHI_1996_S3430090 | [498] |  |
| $B$ fragmentation | DELPHI_2002_069_CONF_603 | [500] |  |

Table 16: Observables used in the tune killing exercise.

| Generator and version | Tunes |
| :--- | :--- |
| Sherpa 1.3.1[[146] | Default (CTEQ6.6) |
| Herwig++ 2.5.2[489] | LHC-UE-EE-3 series (LO $* *$ and CTEQ6L1) |
| Pythia 8.150[348] | 4C |
| PYTHIA 6.425[400] | D6T, DW[501], Z2, AMBT1[502], AUET2B (LO $* *$ and CTEQ6L1)[503], |
|  | Perugia 2010[504], Perugia 2011[504], prof- Q $^{2}[451]$ |
| AlpGen[505] + PYTHIA 6.425 $\left(^{*}\right)$ | Same tunes as PYTHIA6. |
|  | Perugia 2011 using matched ME/PS $\Lambda_{\mathrm{QCD}} \cdot[506]$ |
| HERWIG 6.510[488] + JIMMY 4.31[507] | AUET2 LO $* *[508]$ |
| AlpGen + HERWIG 6.5 + JIMMY 4.31 $\left(^{*}\right)$ | Same as for HERWIG+JIMMY. |

Table 17: Generators and tunes used in the tune killing exercise. (*) Jet and $Z$ boson $\phi^{*}$ observables only.
the total bin error, $\operatorname{dev}_{b}=\left(\mathrm{MC}_{b}-\operatorname{data}_{b}\right) / \operatorname{err}_{b}$.
For each active histogram, the system then reports the $\chi^{2} / N_{\text {bin }}$, and the median, mean, and maximum bin-wise deviation. A total "metric" value for each histogram is reported as the maximum bin-wise deviation if that is greater than $10 \sigma$, otherwise the greater of the median and mean deviations. This hybrid treatment of the metric allows the system to flag up histograms in which there are either widespread moderate deviations or a small number of very discrepant bins which might be missed with a pure median or mean deviation treatment. An HTML table and set of histograms are rendered by the system for each observable, with a continuous colour coding scheme used to highlight the relative quality of data description from ideal (green) to very poor (red).
The histograms are grouped to collect together observables from different sources which reflect related aspects of QCD modelling. The current groups are "Underlying Event (UE)", "Dijets", "Multijets", "Jet shapes", "W and Z", "Fragmentation", and " $B$ fragmentation". In these groups, the same $\chi^{2} / N_{\text {bin }}$, and mean/median/maximum deviation statistics are calculated as before. For visual compactness of classification we again use a hybrid performance metric for each histogram group: again this is the maximum bin-wise deviation found in the contained histograms if that is greater than $10 \sigma$, otherwise the maximum histogram-wise deviation metric in the group if that is greater than $5 \sigma$, otherwise the maximum of the median/mean bin-wise deviation.
The Web pages generated to present this data in a compact way consist of a single top level page containing a colour-coded table of tune performance metrics for each histogram group. Each cell in the table is hyperlinked to a more detailed table for that tune/group where the various $\chi^{2} / N$, max/mean/median deviation and hybrid metric are presented, again colour-coded, for each histogram in the group. The table rows are then hyperlinked to a plot page showing explicitly the tune/generator behaviour for each histogram and indicating the active range of the histograms where appropriate. These pages are shown in Figures 111 to 113 . This form of presentation allows a rapid assessment of generator/tune performance, while still permitting detailed investigation of any flagged-up issues with a few mouse clicks. The system is easily extensible to more observables, groups, and different theory uncertainty / visual classification thresholds.
The classification colours for each performance figure are generated in HSB colour space as a linear variation in deviation $x$ between green (120) and red (0) in the Hue parameter, i.e. $H=120(1-$ $\left.\min \left(x / x_{\text {bad }}, 1.0\right)\right)$, with fixed Saturation and Brightness parameters. The visual threshold $x_{\text {bad }}$ was chosen to be different for each metric type: $5 \sigma$ for maximum deviations, $4 \sigma$ for $\chi^{2} / N$, and $2 \sigma$ for mean and median deviations, and for the hybrid performance metrics. These thresholds were iterated from initial suggestions to the point where distinctions could be made between the models: similar iteration of the discriminating criteria are envisaged while significant model/tune variations exist as the motivation of this study is model discrimination rather than passing or failing a natural performance figure.

### 21.3 Results

As the central theme of this project has been to provide a comprehensible visualisation of the relative performance of generators and tunes, and hierarchical presentation via Web pages was key to achieving this, it would be self-defeating to attempt to present the same information in this summary. Additionally, the nature of tune comparison is that it evolves as new data, tunes, and generator versions become available. Hence, for up-to-date status information we refer the reader to the persistent "tune killing" web page at http:/ /projects.hepforge.org/rivet/tunecmp/.
However, it is worth mentioning some of the most striking features of generators which have been made more evident by this collating of data-MC comparisons:

- The general quality of jet and W/Z data description is in fact better than expected: among PYTHIA tunes in particular there is sufficient variation in parton shower parameters that significant deviations in jet observables would reasonably be expected, but in fact the majority of tunes describe


## Tune comparisons

Deviation metrics per gen/tune and observable group:

| Gen | Tune | UE | Dijets | Multijets | Jet shapes | W and Z | Fragmentation | B frag |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AlpGen | HERWIG6 | - | 1.83 | 5.36 | 2.48 | 0.91 | - | - |
|  | PYTHIA6-AMBT1 | - | 1.55 | 2.80 | 0.61 | 0.53 | - | - |
|  | PYTHIA6-D6T | - | 1.38 | 2.67 | 2.31 | 1.67 | - | - |
|  | PYTHIA6-P2010 | - | 1.09 | 2.65 | 2.03 | 1.48 | - | - |
|  | PYTHIA6-P2011 | - | 1.12 | 2.60 | 0.48 | 0.24 | - | - |
|  | PYTHIA6-Z2 | - | 1.48 | 2.63 | 0.55 | 0.48 | - | - |
|  | PYTHIA6-profQ2 | - | 1.16 | 2.65 | 1.43 | 1.29 | - | - |
| HERWIG | AUET2-CTEQ6L1 | 0.43 | 0.55 | 0.77 | 0.35 | 0.58 | 22.80 | 2.38 |
|  | AUET2-LOxx | 0.25 | 0.71 | 0.60 | 0.39 | 0.88 | 22.13 | 2.29 |
| Herwig++ | 2.5.1-UE-EE-3-CTEQ6L1 | 0.27 | 0.87 | 0.78 | 0.51 | 0.98 | 10.58 | 1.32 |
|  | 2.5.1-UE-EE-3-MRSTLOxx | 0.23 | 1.05 | 0.78 | 0.50 | 0.65 | 10.58 | 1.32 |
| PYTHIA6 | AMBT1 | 0.39 | 1.20 | 0.54 | 0.77 | 0.27 | 0.93 | 1.65 |
|  | AUET2B-CTEQ6L1 | 0.16 | 0.92 | 0.44 | 0.59 | 0.74 | 0.67 | 1.29 |
|  | AUET2B-LOxx | 0.13 | 1.33 | 0.55 | 0.58 | 1.15 | 0.67 | 1.30 |
|  | D6T | 0.58 | 0.79 | 0.50 | 0.56 | 1.25 | 0.36 | 2.63 |
|  | DW | 0.81 | 0.78 | 0.61 | 0.56 | 1.33 | 0.36 | 2.63 |
|  | P2010 | 0.30 | 0.93 | 0.82 | 1.07 | 0.30 | 0.44 | 1.75 |
|  | P2011 | 0.12 | 0.89 | 0.67 | 1.02 | 0.53 | 0.43 | 2.13 |
|  | ProfQ2 | 0.51 | 0.67 | 0.81 | 0.51 | 0.64 | 0.30 | 1.65 |
|  | Z2 | 0.18 | 0.94 | 0.73 | 0.80 | 0.30 | 0.95 | 2.78 |
| Pythias | 4 C | 0.30 | 0.97 | 0.93 | 0.50 | 0.90 | 0.38 | 1.12 |
| Sherpa | 1.3.1 | 0.68 | 0.47 | 0.34 | 0.71 | 0.36 | 0.75 | 2.48 |

Fig. 111: Screenshot of the top-level summary page produced by the tune comparison system.
Jet shapes

| Histo | chi2/Nat | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Jet shape svinos for Sp_\.... (ATLAS_2011_S8924791/d01-x06-y01) | 0.59 | 0.77 | 0.69 | 1.17 | 0.77 |
| jet shape Svihos for Sp_lp... (ATLAS_2011_58924791/d09-×06-y01) | 0.14 | 0.36 | 0.30 | 0.61 | 0.36 |
| Central Transv. Thrust, $59 \ldots$ (CMS_2011_ $58957746 / 101 \times \times 01$-y01) | 0.37 | 0.43 | 0.53 | 1.08 | 0.53 |
| Central Transv. Minor, 590... (CMS_2011_58957746/d02-x01-y01) | 0.34 | 0.38 | 0.48 | 1.14 | 0.48 |

## W and Z

| Histo | chi2/Ndf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Muon channel ( $\mathrm{s} \mid \mathrm{y}$ _ $\mathrm{Z} \mid<1 \mathrm{~s}$ ) (D0_2010_ $58821313 / 802$-x01-y01) | 0.77 | 0.70 | 0.79 | 1.52 | 0.79 |
| Muon channel ( $\$ 1<\mid y \mathrm{z}$ Z\|<2s) (00_2010_s8821313/d02-x01-y02) | 0.27 | 0.38 | 0.45 | 1.08 | 0.45 |

## Fragmentation

| Histo | chi2/Wdf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Scaled momentum, 5x.p = \|p... (DELPH1_1996_S3430090/d07-x01-y01) | 0.74 | 0.28 | 0.47 | 3.29 | 0.47 |
| S1-text(Thrust)s (DELPHI_1996_S3430090/d11-x01-y01) | 4.12 | 0.24 | 1.13 | 8.26 | 1.13 |
| Thrust major, SMS (DELPH1_1996_53430090/d12-x01-y01) | 7.24 | 0.50 | 1.61 | 9.37 | 1.61 |
| Thrust minor, sms (DELPH1_1996_53430090/d13-x01-y01) | 9.69 | 0.40 | 1.57 | 10.58 | 10.58 |
| Mean charged mutitilicity (DELPH1_1996_S3430090/d35-x01-y01) | 0.08 | 0.28 | 0.28 | 0.28 | 0.28 |

Fig. 112: Screenshot of the mid-level performance metric page produced by the tune comparison system. This specific example is part of the performance metrics for the Herwig++ LHC-UE-EE-3 LO $* *$ tune.

## Plots for PYTHIA6, AUET2B-LOxx, B frag



Fig. 113: Screenshot of the observable plot page produced by the tune comparison system. This specific example shows the $B$ fragmentation performance of the PYTHIA6 AUET2B LO** tune.
data fairly well.

- The UE in particular has been a focus of tuning activity and this is evident in the consistency of UE data description. The worst performance in this group is from the DW tune of PYTHIA, but even this pre-LHC tune with the "old" PYTHIA MPI model achieves a deviation metric of less than $1 \sigma$ on LHC UE observables.
- PYTHIA D6T outperforms PYTHIA DW - an unexpected result since the MPI energy evolution of D6T is fixed to the default and disfavoured form $p_{\perp}^{0}(s) \sim(\sqrt{s} / 1800 \mathrm{GeV})^{0.16}$, whereas the exponent in DW is closer to the tuned consensus of $\sim 0.25$. This may be a lucky behaviour at 7 TeV , and hence care is needed with extrapolation of D6T to 8,10 , or 14 TeV , but it is clear that the PYTHIA $Q^{2}$-ordered parton shower is not yet dead on purely physics grounds. The best tune of this PYTHIA configuration, however, is Prof- $Q^{2}$, which in addition to general small improvements, is significantly better than DW or D6T at describing the vector boson $p_{\perp}$ distribution.
- Pythia8 is generally seen to perform very well, and provides significant improvements over PYTHIA6 for jet shapes and $B$ fragmentation. Tuning focus is accordingly beginning to shift towards Pythia8, also for minimum bias observables not yet considered here.
- AlpGen interacts strongly with tunes on jet shape and vector boson data descriptions. In particular there appears to be little motivation to use AlpGen with the D6T or Perugia 2010 tunes of PYTHIA6. AlpGen+HERWIG also has significant problems with jet shapes in particular, and the indication of this study is that AlpGen+PYTHIA Perugia 2011 is the most performant configuration, closely followed by AlpGen+PYTHIA Z2. Notably, the Perugia 2011 tune of PYTHIA was specifically developed to minimise ME/PS merging artefacts when used with AlpGen.
- Both HERWIG and Herwig++ have problems describing LEP fragmentation data, but Herwig++ is a very significant improvement over its Fortran cousin. The identified hadron rates are in particular much improved, although $K^{ \pm}$and $\Sigma^{0}$ remain anomalous. However, a known problem with Herwig++ is the poor description of the LEP thrust distribution, which overshoots significantly in the multi-parton region.
- AlpGen seems to have difficulty describing dijet azimuthal decorrelations, even when restricted to the $2 / 3$ parton region of the plot. This is particularly surprising as AlpGen is intended to provide
the multi-parton configurations needed to describe this observable.
- $B$ fragmentation is in general quite poorly described. The best descriptions are by Pythia8, the AUET2B tunes of PYTHIA6, and Herwig++. Other generators and tunes are in decidedly dodgy shape for $B$-specific predictions at the LHC.
Insofar as it is within the scope of this project to make recommendations for canonical generator and tune choices, we note that the Perugia 2011, AUET2B, and Z 2 tunes of PYTHIA6 provide the best data descriptions currently available with that generator and that the Prof- $Q^{2}$ tune is the best available configuration using the $Q^{2}$-ordered PYTHIA parton shower. We hence recommend these 4 PYTHIA tunes as the current minimal set of PYTHIA tunes for general use at the LHC, particularly once an update of the ATLAS AUET2B tune has fixed the tuning issue with the $Z p_{\perp}$.
Among the other generators, where there is not such a proliferation of tunes, we note again the apparent performance issues with AlpGen - this is clearly in need of further pursuit. However, to reduce the amount of comparison needed, we note that Perugia 2011 is the only PYTHIA6 tune now optimised for use with AlpGen with avoidance of the worst effects of ME/PS coupling mismatches: hence future studies can quite happily restrict themselves to this AlpGen+PYTHIA configuration. As AlpGen+HERWIG has several problems with jet description, HERWIG itself has serious problems with both light and $B$ fragmentation, and no further tuning of the JIMMY MPI model is envisaged, the HERWIG generator cannot be recommended for future use in any capacity where an alternative exists.
The "new" C++ generators Herwig++, Pythia8, and Sherpa all perform well, with the exception of Sherpa's $B$ fragmentation and the Herwig++ light fragmentation. Pythia8 generally behaves well but some tuning or development may be needed to improve inter-jet observables and the $Z p_{\perp}$ spectrum. In general, the $\mathrm{C}++$ generators are in good health, and we anticipate further improvements as the focus of tuning studies shifts to them.


### 21.4 Outlook

This project has put in place a system and a set of classification criteria which have proven useful for summarising and investigating MC generator model and tune predictivity for a variety of QCD phenomena. While we claim no mandate to truly "kill" certain tunes or generators, and wish to emphasise that a poor performance in a single observable type (in particular $B$ fragmentation) certainly does not render that generator useless, the results from these comparisons do provide strong arguments for deprecation of at least several PYTHIA6 tunes and of the Fortran HERWIG generator in general.
It is the nature of a project like this that results are continually being updated, and there are many natural avenues for extension which we wish to pursue, in particular:

- Extra observables, e.g. minimum bias and $E_{\perp}$ flow, LHC and Tevatron photon physics, LHC $W / Z$ $p_{\perp}$ data, strangeness data from LHC and RHIC, explicit multijet observables, etc..
- Extra generators and tunes, in particular POWHEG+PYTHIA/HERWIG/Pythia8/Herwig++, MadGraph+PYTHIA/Pythia8, MC@NLO+HERWIG/Herwig++. Comparison between Sherpa with the CTEQ6.6 and CTEQ6L1 PDFs. New Pythia8 and PYTHIA6 tunes from ATLAS.
Greater automation of the data generation will be important, as finding resources (human rather than $\mathrm{CPU}!$ ) to produce and run combinatoric numbers of generator/tune/PDF/observable combinations has been troublesome. We suggest that this project can make use of the output of the CERN LPCC MCplots system (also Rivet-based) for future extension. We also look forward to a forthcoming major upgrade of the Rivet histogramming system which will greatly simplify the treatment of multi-leg generators for which the $n$-parton samples must be explicitly merged, e.g. AlpGen, MadGraph, etc.


## 22. COMPACT ASCII OUTPUT FORMAT FOR HEPMC 59

## Abstract

[^165]We discuss the possibility of reducing the footprint of HepMC event files. Different compression options are discussed, and a suggestion for an update of the HepMC ASCII file format is presented.

### 22.1 Introduction

The HepMC [509] event record has become the de-facto standard for communicating events between event generators and different kinds of analysis programs. HepMC also provides an ASCII-based file format for storing and retrieving events to and from disk, which has also become the standard. This file format is not at all optimized for size, and although disk space today is fairly cheap, there are still problems associated with handling very large files.
A typical minimum-bias 7 TeV LHC HepMC event occupies around 50 kB when written on disk. More interesting events are usually bigger than this and one would typically want to store many events to get anywhere near the statistics collected by any of the LHC experiments; it is clear that such event files will become very large and difficult to handle. Even with standard compression algorithms such as gzip and bzip2, where these file sizes can be reduced by a factor 3 or more, the problem is still substantial.
One could imagine using a binary output format to reduce the event size. Writing a 4 byte floating point number in an ASCII file typically takes 10-12 characters, so here one could expect to reduce file sizes up to a factor 3 . However, standard compression algorithms are rather good at identifying strings of numbers and compressing them, so there is normally not much to be gained by using a compressed binary format compared to a compressed ASCII one. In addition one would lose the advantage of ASCII files that they are (somewhat) readable to the human eye.
Instead the key to reducing file sizes is to remove redundant and unnecessary information stored in the files. This could involve completely reversible operations such as removing the information about the momentum of an intermediate particle, as this can be reconstructed from its decay products. It could also involve irreversible operations such as reducing the precision on the momenta. In the following we describe a number of such operations, which allows us to reduce the file sizes by almost a factor 30 .

### 22.2 The Benchmarking procedure

We started out by generating 1000 non-diffractive QCD events with Pythia 6.425[400] using the AGILe [360] interface. The resulting file size was 48 MB , which can be reduced to 16 MB or 13 MB using gzip or bzip2 respectively. We then investigated several ways of reducing this size.

Removing irrelevant particles The HepMC format contains quite a lot of information about how the event was generated, such as intermediate particles in the hard sub process, which may be generatordependent (and often unphysical) and is not relevant when comparing to experimental data. In principle one could argue that the only thing that should be written out is final-state stable particles (with HepMC status code 1). However, there are circumstances where information about intermediate unstable hadrons (status code 2) is relevant. The AGILe event generator interface already includes facilities for keeping only particle entries with status code 1 or 2.

Reconstructible information Some information in the HepMC file is redundant in the sense that it can be reconstructed from other information in the file. Here are some examples.

- Both energy, momentum and invariant mass of each particle is written out. Clearly, we can eg. reconstruct the energy given the three-momentum and mas $5^{60}$.

[^166]| Format | Status codes | no comp. <br> (MB) | gzip <br> (MB) | bzip2 <br> (MB) |
| :--- | ---: | ---: | ---: | ---: |
| Standard | All | 48 | 16 | 13 |
|  | $1 \& 2$ | 43 | 15 | 13 |
|  | 1 | 17 | 6.0 | 4.8 |
| Compact | All | 18 | 3.3 | 2.1 |
|  | $1 \& 2$ | 13 | 2.9 | 1.9 |
|  | 1 | 4.0 | 1.9 | 1.6 |
| Compact binary | 1 | 1.8 | 1.7 | 1.7 |

Table 18: Size of the benchmark file after applying different compression methods.

- The three-momenta of decayed hadrons (status code 2 ) can be reconstructed from the sum of the momenta of the decay products.
- The mass of a stable particle can be deduced from the particle ID.
- The position of a vertex can be deduced from the previous vertex position and the life-time and momentum direction of the connecting particle.
- Each particle in a HepMC event has a unique bar code, which is an otherwise arbitrary integer. No loss of information would result from renumbering the particles, simply inferring their bar code from the order in which they appear in the event.

Precision Clearly, having 8 byte floating point numbers is not very relevant for many of the numbers in an event file. When comparing with experimental data, there is no point in having much larger precision than what is achievable in the experiment, and it makes sense to match the the information in the HepMC file to the precision of the actually measured variables in the experiments.
A possible example is to store masses and transverse momenta as integers in units of 0.1 MeV , azimuthal angles as integers in units of $0.00002 \times \pi$, pseudorapidities as integers in units of 0.00001 and vertex positions as integers in units of 0.001 mm .

### 22.3 Benchmark Results

We have investigated several of the options listed in the previous section, and the resulting file sizes when applied to the benchmark file is presented in table 18 . Firstly we see the size reduction using the standard format and simply reducing the number of particles, keeping only those with status code 2 and 1 or only 1 . Next we present the same results, but using a compact format which keeps the structure of the HepMC ASCII file but applies all optimizations discussed above. Finally, for reference, we present an aggressively compacted Binary format which uses the following optimizations for each particle: stores 1 float for transverse and 1 float for longitudinal momentum, a 3-byte integer for phi, and 1 byte for PDG IDs (rare PDG IDs are written out with 4 full bytes). This format loses the HepMC structure of the event and in some sense this represents the target size, below which it is difficult to go.
It is clear that one does not gain much by using a binary format provided one uses the optimizations presented above together with bzip2 compression algorithm.

### 22.4 Outlook

Given the results above, the work to include a more efficient file format for the HepMC has begun. The suggestion is to keep the current structure of the file format, but to add options to exclude all particles except those with status code 1 (or 2). Furthermore options for the representation and precision of momenta and vertex positions will be included as well as options for excluding (simply replacing with a single exclamation mark for easy parsing) information which can be reconstructed. The new format will be included in a forthcoming HepMC version during 2012.

In this report we have not looked carefully at the time it takes to read the different formats. With the default HepMC format this can be many times larger than the time taken for typical particle-level analyses, while for minimal binary formats it is of the same order. We defer detailed study of this question to future work.

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# HEAVY QUARK PRODUCTION IN THE ACOT SCHEME BEYOND NLO* 

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We compute the structure functions $F_{2}$ and $F_{\mathrm{L}}$ in the ACOT scheme for heavy quark production. We use the complete ACOT results to NLO, and make use of the $\overline{\mathrm{MS}}$ massless results at NNLO and $\mathrm{N}^{3} \mathrm{LO}$ to estimate the higher order mass-dependent corrections. We show numerically that the dominant heavy quark mass effects can be taken into account using massless Wilson coefficients together with an appropriate rescaling prescription. Combining the exact NLO ACOT scheme with these expressions should provide a good approximation to the full calculation in the ACOT scheme at NNLO and $\mathrm{N}^{3} \mathrm{LO}$.

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## 1. Introduction

The production of heavy quarks in high energy processes has become an increasingly important subject of study both theoretically and experimentally. The theory of heavy quark production in perturbative Quantum Chromodynamics (pQCD) is more challenging than that of light parton (jet) production because of the new physics issues brought about by the additional heavy quark mass scale. The correct theory must properly take into account the changing role of the heavy quark over the full kinematic range of the relevant process from the threshold region (where the quark behaves like

[^167]a typical "heavy particle") to the asymptotic region (where the same quark behaves effectively like a parton, similar to the well known light quarks $\{u, d, s\}$ ).

With the ever-increasing precision of experimental data and the progression of theoretical calculations and parton distribution function (PDF) evolution to next-to-next-to-leading order (NNLO) of QCD, there is a clear need to formulate and also implement the heavy quark schemes at this order and beyond. The most important case is arguably the heavy quark treatment in inclusive deep-inelastic scattering (DIS) since the very precise HERA data for DIS structure functions and cross sections form the backbone of any modern global analysis of PDFs. Here, the heavy quarks contribute up to $30 \%$ or $40 \%$ to the structure functions at small momentum fractions $x$. Extending the heavy quark schemes to higher orders is, therefore, necessary for extracting precise PDFs , and this is a prerequisite for precise predictions of observables at the LHC. However, we would like to also stress the theoretical importance of having a general pQCD framework that includes heavy quarks and is valid to all orders in perturbation theory over a wide range of hard energy scales.

An example, where higher order corrections are particularly important is the structure function $F_{\mathrm{L}}$ in DIS. The leading order $\left(\mathcal{O}\left(\alpha_{\mathrm{S}}^{0}\right)\right)$ contribution to this structure function vanishes for massless quarks due to helicity conservation (Callan-Gross relation). This has several consequences: (1) $F_{\mathrm{L}}$ is useful for constraining the gluon PDF via the dominant subprocess $\gamma^{*} g \rightarrow q \bar{q}$. (2) The heavy quark mass effects of order $\mathcal{O}\left(\frac{m^{2}}{Q^{2}}\right)$ are relatively more pronounced ${ }^{1}$. (3) Since the first non-vanishing contribution to $F_{\mathrm{L}}$ is next-to-leading order (up to mass effects), the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ corrections are more important than for $F_{2}$. In Fig. 1, we show a comparison of different theoretical calculations of $F_{\mathrm{L}}$ with preliminary HERA data [2]. As can be seen, in particular at small $Q^{2}$ (i.e. small $x$ ), there are considerable differences between the predictions.

The purpose of this paper is to calculate the leading twist neutral current DIS structure functions $F_{2}$ and $F_{\mathrm{L}}$ in the ACOT factorization scheme up to order $\mathcal{O}\left(\alpha_{\mathrm{S}}^{3}\right)\left(\mathrm{N}^{3} \mathrm{LO}\right)$ and to estimate the error due to approximating the heavy quark mass terms $\mathcal{O}\left(\alpha_{\mathrm{S}}^{2} \times \frac{m^{2}}{Q^{2}}\right)$ and $\mathcal{O}\left(\alpha_{\mathrm{S}}^{3} \times \frac{m^{2}}{Q^{2}}\right)$ in the higher order corrections. The results of this study form the basis for using the ACOT scheme in NNLO global analyses and for future comparisons with precision data for DIS structure functions.

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Fig. 1. $F_{\mathrm{L}}$ vs. $Q$ from combined HERA-I inclusive deep inelastic cross sections measured by the H1 and ZEUS collaborations. Figure taken from Ref. [2].

This paper is organized as follows. In Sec. 2, we review theoretical approaches to include heavy flavors in QCD calculations. Particular emphasis is put on the ACOT scheme which is a minimal extension of the $\overline{\mathrm{MS}}$ scheme. In Sec. 3, we present the prescription for constructing the approximate DIS structure functions in the ACOT scheme up to $\mathcal{O}\left(\alpha_{S}^{3}\right)$ order. The corresponding numerical results are presented in Sec. 4. Finally, in Sec. 5 we summarize the main results. This work is based on Ref. [3], and further details can be found therein.

## 2. Review of theoretical methods

We review theoretical methods which have been advanced to improve existing QCD calculations of heavy quark production, and the impact on recent experimental results.

### 2.1. ACOT Scheme

The ACOT renormalization scheme $[4,5]$ provides a mechanism to incorporate the heavy quark mass into the theoretical calculation of heavy quark production both kinematically and dynamically. In 1998, Collins [6] extended the factorization theorem to address the case of heavy quarks; this work provided the theoretical foundation that allows us to reliably compute heavy quark processes throughout the full kinematic realm.

If we consider the DIS production of heavy quarks at $\mathcal{O}\left(\alpha_{\mathrm{S}}^{1}\right)$ this involves the LO $Q V \rightarrow Q$ process and the NLO $g V \rightarrow Q \bar{Q}$ process $^{2}$. The key ingredient provided by the ACOT scheme is the subtraction term (SUB) which removes the "double counting" arising from the regions of phase space, where the LO and NLO contributions overlap. Specifically, at NLO order, we can express the total result as a sum of

$$
\begin{equation*}
\sigma_{\mathrm{TOT}}=\sigma_{\mathrm{LO}}+\left\{\sigma_{\mathrm{NLO}}-\sigma_{\mathrm{SUB}}\right\}, \tag{1}
\end{equation*}
$$

where the subtraction term for the gluon-initiated processes is

$$
\begin{equation*}
\sigma_{\mathrm{SUB}}=f_{g} \otimes \tilde{P}_{g \rightarrow Q} \otimes \sigma_{Q V \rightarrow Q} \tag{2}
\end{equation*}
$$

$\sigma_{\text {SUB }}$ represents a gluon emitted from a proton $\left(f_{g}\right)$ which undergoes a collinear splitting to a heavy quark $\left(\tilde{P}_{g \rightarrow Q}\right)$ convoluted with the LO quarkboson scattering $\sigma_{Q V \rightarrow Q}$. Here, $\tilde{P}_{g \rightarrow Q}(x, \mu)=\frac{\alpha_{\mathrm{S}}}{2 \pi} \ln \left(\mu^{2} / m^{2}\right) P_{g \rightarrow Q}(x)$, where $P_{g \rightarrow Q}(x)$ is the usual $\overline{\text { MS }}$ splitting kernel, $m$ is the quark mass and $\mu$ is the renormalization scale which we typically choose to be $\mu=Q$.

An important feature of the ACOT scheme is that it reduces to the appropriate limit both as $m \rightarrow 0$ and $m \rightarrow \infty$ as we illustrate below. Specifically, in the limit where the quark $Q$ is relatively heavy compared to the characteristic energy scale $(\mu \lesssim m)$, we find $\sigma_{\mathrm{LO}} \sim \sigma_{\mathrm{SUB}}$ such that $\sigma_{\mathrm{TOT}} \sim \sigma_{\mathrm{NLO}}$. In this limit, the ACOT result naturally reduces to the Fixed-Flavor-NumberScheme (FFNS) result. In the FFNS, the heavy quark is treated as being extrinsic to the hadron, and there is no corresponding heavy quark PDF ( $f_{Q} \sim 0$ ); thus $\sigma_{\mathrm{LO}} \sim 0$. We also have $\sigma_{\mathrm{SUB}} \sim 0$ because this is proportional to $\ln \left(\mu^{2} / m^{2}\right)$. Thus, when the quark $Q$ is heavy relative to the characteristic energy scale $\mu$, the ACOT result reduces to $\sigma_{\text {TOT }} \sim \sigma_{\text {NLO }}$.

Conversely, in the limit where the quark $Q$ is relatively light compared to the characteristic energy scale ( $\mu \gtrsim m$ ), we find that $\sigma_{\text {LO }}$ yields the dominant part of the result, and the "formal" $\mathrm{NLO} \mathcal{O}\left(\alpha_{\mathrm{S}}\right)$ contribution $\left\{\sigma_{\mathrm{NLO}}-\sigma_{\mathrm{SUB}}\right\}$ is an $\mathcal{O}\left(\alpha_{\mathrm{S}}\right)$ correction. In this limit, the ACOT result will reduce to the MS Zero-Mass Variable-Flavor-Number-Scheme (ZM-VFNS) limit exactly without any finite renormalizations. The quark mass $m$ no longer plays any dynamical role and purely serves as a regulator. The $\sigma_{\text {NLO }}$ term diverges due to the internal exchange of the quark $Q$, and this singularity is canceled by $\sigma_{\text {SUB }}$.

We illustrate the versatile role of the quark mass in Fig. 2 (a), where we display $F_{2}^{c}$ as a function of $Q$ calculated in the ZM-VFNS, FFNS, ACOT, and S-ACOT schemes. We see that the ACOT scheme coincides with the

[^169]FFNS for small $Q$, and the ZM-VFNS for large $Q$. In Fig. $2(\mathrm{~b})$, we plot $F_{2}^{c}$ as a function of the quark mass $m$ for a fixed $Q=10 \mathrm{GeV}$ for the MS ZM-VFNS and ACOT schemes. We observe that when $m$ is within a decade or two of $\mu$, the quark mass plays a dynamic role; however, for $m \ll \mu$, the quark mass purely serves as a regulator and the specific value is not important. Operationally, it means we can obtain the $\overline{\mathrm{MS}} \mathrm{ZM}-V F N S$ result either by (i) computing the terms using dimensional regularization and setting the regulator to zero, or (ii) by computing the terms using the quark mass as the regulator and then setting this to zero.


Fig. 2. (a) $F_{2}^{c}$ for $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number Scheme (FFNS), and Zero-Mass Variable Flavor Number Scheme (ZM-VFNS). The ACOT and S-ACOT results are virtually identical. (b) Comparison of $F_{2}^{c}(x, Q)$ (scaled by $10^{4}$ ) vs. the quark mass $m$ in GeV for fixed $x=0.1$ and $Q=10 \mathrm{GeV}$. The full (red) dots are the full ACOT result, and the solid (blue) line is the massless $\overline{\mathrm{MS}}$ result.

The ACOT scheme is minimal in the sense that the construction of the massive short distance cross sections does not need any observabledependent extra contributions or any regulators to smooth the transition between the high and low scale regions. The ACOT prescription is: (a) calculate the massive partonic cross sections, and (b) perform the factorization using the quark mass as regulator.

It is in this sense that we claim the ACOT scheme is the minimal massive extension of the $\overline{\mathrm{MS}}$ ZM-VFNS. In the limit $m / \mu \rightarrow 0$ it reduces exactly to the $\overline{\mathrm{MS}} \mathrm{ZM}-V F N S$, in the limit $m / \mu \gtrsim 1$ the heavy quark decouples from the PDFs and we obtain exactly the FFNS for $m / \mu \gg 1$ and no finite renormalizations are needed.

### 2.2. S-ACOT

In a corresponding application, it was observed that the heavy quark mass could be set to zero in certain pieces of the hard scattering terms without any loss of accuracy. This modification of the ACOT scheme goes by the name Simplified-ACOT (S-ACOT) and can be summarized as follows [8].

S-ACOT: For hard-scattering processes with incoming heavy quarks or with internal on-shell cuts on a heavy quark line, the heavy quark mass can be set to zero $(m=0)$ for these pieces.

If we consider the case of NLO DIS heavy quark production, this means we can set $m=0$ for the LO terms $\sigma_{Q V \rightarrow Q}$ (incoming heavy quark), and for the SUB terms (on-shell cut on an internal heavy quark line). Hence, the only contribution which requires calculation with $m$ retained is the NLO $g V \rightarrow Q \bar{Q}$ process. Figure 2 (a) displays a comparison of a calculation using the ACOT scheme with all masses retained vs. the S-ACOT scheme; as expected, these two results match throughout the full kinematic region.

It is important to note that the S-ACOT scheme is not an approximation; this is an exact renormalization scheme, extensible to all orders.

### 2.3. ACOT and $\chi$-rescaling

As we have illustrated in Sec. 2.1, in the limit $Q^{2} \gg m^{2}$ the mass simply plays the role of a regulator. In contrast, for $Q^{2} \sim m^{2}$ the value of the mass is of consequence for the physics. The mass can enter dynamically in the hard-scattering matrix element, and can enter kinematically in the phase space of the process.

We will demonstrate that for the processes of interest the primary role of the mass is kinematic and not dynamic. It was this idea which was behind the original slow-rescaling prescription of [9] which considered DIS charm production (e.g., $\gamma c \rightarrow c$ ) introducing the shift $x \rightarrow \chi=x\left[1+\left(m_{c} / Q\right)^{2}\right]$. This prescription accounted for the charm quark mass by effectively reducing the phase space for the final state by an amount proportional to $\left(m_{c} / Q\right)^{2}$.

This idea was extended in the $\chi$-scheme by realizing that (in most cases) in addition to the observed final-state charm quark, there is also an anticharm quark in the beam fragments since all the charm quarks are ultimately produced by gluon splitting $(g \rightarrow c \bar{c})$ into a charm pair. For this case, the scaling variable becomes $\chi=x\left[1+\left(2 m_{c} / Q\right)^{2}\right]$. This rescaling is implemented in the $\mathrm{ACOT}_{\chi}$ scheme, for example $[10,11,12]^{3}$. The factor $\left(1+\left(2 m_{c}\right)^{2} / Q^{2}\right)$ represents a kinematic suppression factor which will suppress the charm process relative to the lighter quarks. Additionally, the $\chi$-scaling ensures the threshold kinematics ( $W^{2}>4 m^{2}+M^{2}$ ) is satisfied; while it is important to satisfy this condition for large $x$, this may prove too restrictive at small $x$, where the HERA data are especially precise.

[^170]To encompass all the above results, we can define a general scaling variable $\chi(n)$ as

$$
\begin{equation*}
\chi(n)=x\left[1+\left(\frac{n m_{c}}{Q}\right)^{2}\right] \tag{3}
\end{equation*}
$$

where $n=\{0,1,2\}$. Here, $n=0$ corresponds to the massless result without rescaling, $n=1$ corresponds to the original Barnett slow-rescaling, and $n=2$ corresponds to the $\chi$-rescaling.

### 2.4. Phase space (kinematic) and dynamic mass

We now investigate the effects of separately varying the mass entering the $\chi(n)$ variable taking into account the phase space constraints and the mass value entering the hard scattering cross section $\widehat{\sigma}(m)$. We call the former mass parameter "phase space (kinematic) mass" and the latter "dynamic mass".


Fig. 3. Comparison of phase space (kinematic) and dynamic mass effects. (a) Comparison of $F_{2}^{c}(x, Q)$ vs. $Q$ for the NLO ACOT calculation for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) using zero dynamic mass $[\widehat{\sigma}(m=0)]$ to show the effect of $n$ scaling; from top to bottom $n=\{0,1,2\}$ (pink, black, purple). (b) Comparison of $F_{2}^{c}(x, Q)$ vs. $Q$ for the NLO ACOT calculation for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). Here we keep the scaling fixed $n=2$ and compare the effect of varying the dynamic mass in the Wilson coefficient. The upper (cyan) curve uses a non-zero dynamic mass $[\widehat{\sigma}(m=1.3)]$ and the lower (purple) curve uses a zero dynamic mass $[\widehat{\sigma}(m=0)]$.

In Fig. $3(\mathrm{a})$, we display $F_{2}^{c}(x, Q)$ vs. $Q$. The family of 3 curves shows the NLO ACOT calculation with $\chi(n)$ scaling using a zero dynamic mass for the hard scattering. We compare this with Fig. 3 (b) which shows $F_{2}^{c}(x, Q)$ in the NLO ACOT scheme using a fixed $n=2$ scaling, but varying the mass used in the hard-scattering cross section. The upper (cyan) curves use a nonzero dynamic mass $\left[\widehat{\sigma}\left(m_{c}=1.3\right)\right]$ and the lower (purple) curves have been obtained with a vanishing dynamic mass $\left[\widehat{\sigma}\left(m_{c}=0\right)\right]$. We observe that the effect of the "dynamic mass" in $\widehat{\sigma}\left(m_{c}\right)$ is only of consequence in the limited region $Q \gtrsim m$, and even in this region the effect is minimal. In contrast, the influence of the phase space (kinematic) mass shown in Fig. 3 (a) is larger than the dynamic mass shown in Fig. 3 (b).

In conclusion, we have shown that (up to $\mathcal{O}\left(\alpha_{\mathrm{S}}\right)$ ) the phase space mass dependence is generally the dominant contribution to the DIS structure functions. Assuming that this observation remains true at higher orders, it is possible to obtain a good approximation of the structure functions in the ACOT scheme at NNLO and $\mathrm{N}^{3} \mathrm{LO}$ using the massless Wilson coefficients together with a non-zero phase space mass entering via the $\chi(n)$-prescription.

### 2.5. Other massive schemes

There are a number of other schemes for incorporating the heavy quark mass terms, and we briefly note a few examples. The Thorne-Roberts (TR) scheme $[14,15]$ and its derivatives (TR') are designed to provide a smooth threshold behavior, and this is implemented by including pieces of the higher order contributions. The FONLL scheme [16] was originally developed to match fixed order calculations with resumed ones in the case of heavy quark hadroproduction; this approach has been generalized and applied to other applications including DIS structure functions [17]. Details and comparisons of these approached is outlined in the 2009 Les Houches Workshop report [18].

## 3. ACOT scheme beyond NLO

In Sec. 2.4, we have shown using the NLO full ACOT scheme that the dominant mass effects are those coming from the phase space which can be taken into account via a generalized slow-rescaling $\chi(n)$-prescription. Assuming that a similar relation remains true at higher orders one can construct the following approximation to the full ACOT result up to $\mathrm{N}^{3} \mathrm{LO}\left(\mathcal{O}\left(\alpha_{\mathrm{S}}^{3}\right)\right)$

$$
\begin{equation*}
\operatorname{ACOT}\left[\mathcal{O}\left(\alpha_{\mathrm{S}}^{0+1+2+3}\right)\right] \simeq \operatorname{ACOT}\left[\mathcal{O}\left(\alpha_{\mathrm{S}}^{0+1}\right)\right]+\mathrm{ZM}^{-\operatorname{VFNS}_{\chi}}\left[\mathcal{O}\left(\alpha_{\mathrm{S}}^{2+3}\right)\right] \tag{4}
\end{equation*}
$$

Here, the massless Wilson coefficients at $\mathcal{O}\left(\alpha \alpha_{\mathrm{S}}^{2}\right)$ and $\mathcal{O}\left(\alpha \alpha_{\mathrm{S}}^{3}\right)$ are substituted for the Wilson coefficients in the ACOT scheme as the corresponding massive coefficients have not yet been computed.

There has been a calculation of neutral current electroproduction (equal quark masses, vector coupling) of heavy quarks at this order by Smith and van Neerven [19] in the FFNS which could be used to obtain the massive Wilson coefficients in the S-ACOT scheme by applying appropriate collinear subtraction terms ${ }^{4}$; however, this is beyond the scope of this paper. For charge current case massive calculations are available at order $\mathcal{O}\left(\alpha \alpha_{\mathrm{S}}\right)$ [21, 22, 23] and partial results at order $\mathcal{O}\left(\alpha \alpha_{\mathrm{S}}^{2}\right)$ [24].

Here, we argue that the massless Wilson coefficients at $\mathcal{O}\left(\alpha \alpha_{\mathrm{S}}^{2}\right)$ together with a $\chi(n)$-prescription provide a very good approximation of the exact result. At worst, the maximum error would be of order $\mathcal{O}\left(\alpha \alpha_{S}^{2} \times\left[\mathrm{m}^{2} / Q^{2}\right]\right)$. However, based on the arguments of Sec. 2.4 we expect the inclusion of the phase space mass effects to contain the dominant higher order contributions so that the actual error should be substantially smaller.

The massless higher order coefficient functions for the DIS structure function $F_{2}$ via photon exchange can be found in Refs. [25, 26, 27, 28, 29, $30,31,32,33,34]$. The expressions for the structure function $F_{\mathrm{L}}$ have been calculated in Refs. [35, 29, 31, 36, 33].

We now consider our choice for the appropriate generalized $\chi(n)$-rescaling variable. For the purposes of this study, we will vary the phase space mass using the $\chi(n)$ rescaling with $n=\{0,1,2\}$. While $n=0$ corresponds to the massless case (no rescaling), it is not obvious whether $n=1$ or $n=2$ is the preferred rescaling choice for higher orders. Thus, we will use the range between $n=1$ and $n=2$ as a measure of our theoretical uncertainty arising from this ambiguity.

## 4. Results

We now present our results for the $F_{2}$ and $F_{\mathrm{L}}$ structure functions calculated at $\mathrm{N}^{3} \mathrm{LO}$ in the extended ACOT scheme. The initial PDFs, based on the Les Houches benchmark set [37] are evolved using the QCDNUM program [38]. In the calculation we set $m_{c}=1.3 \mathrm{GeV}, m_{b}=4.5 \mathrm{GeV}$ and $\alpha_{\mathrm{S}}\left(M_{Z}\right)=0.118$.

In figures 4 (a) and $4(\mathrm{~b})$, we display the structure functions $F_{2}$ and $F_{\mathrm{L}}$, respectively, for selected $x$ values as a function of $Q$. Each plot has three curves which are computed using $n$-scalings of $\{0,1,2\}$. We observe that the effect of the $n$-scaling is negligible except for very small $Q$ values. This result is in part because the heavy quarks are only a fraction of the total structure function, and the effects of the $n$-scaling are reduced at larger $Q$ values.

[^171]

Fig. 4. $F_{2, \mathrm{~L}}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). The three lines show the scaling variable: $n=\{0,1,2\}$ (red, green, blue). We observe the effect of the $n$-scaling is negligible except for very small $Q$ values. (a) $F_{2}$ vs. $Q$. (b) $F_{\mathrm{L}}$ vs. $Q$.

In Ref. [3] we magnify the small $Q$ region of $F_{\mathrm{L}}$ of Fig. 4 (b) for $x=10^{-5}$, where the effects of using different scalings are largest. We can see that for inclusive observables, the $n=1$ and $n=2$ scalings give nearly identical results, but they differ from the massless case $(n=0)$. This result, together with the observation that at NLO kinematic mass effects are dominant, suggests that the error we have in our approach is relatively small and approximated by the band between $n=1$ and $n=2$ results.

We can investigate the effects of the $\chi(n)$-scaling in more details by examining the flavor decomposition of the structure functions. In figures 5 (a) and $5(\mathrm{~b})$, we display the fractional contributions of quark flavors to the structure functions $F_{2, \mathrm{~L}}$ for selected $n$-scaling values as a function of $Q$. We observe the $n$-scaling reduces the relative contributions of charm and bottom at low $Q$ scales. For example, without any $n$-scaling $(n=0)$ we find the charm and bottom quarks contribute an unusually large fraction at very low scales $\left(Q \sim m_{c}\right)$ as they are (incorrectly) treated as massless partons in this region. The result of the different $n$-scalings $(n=1,2)$ is to introduce a kinematic penalty which properly suppresses the contribution of these heavy quarks in the low $Q$ region. In the following, we will generally use the $n=2$ scaling for our comparisons.


Fig. 5. Effect of $\chi(n)$-scaling for $n=\{0,1,2\}$ (left to right) at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-3}\right\}$. Reading from the bottom, we have fractional contribution for each (final-state) quark flavor to $F_{2, \mathrm{~L}}^{j} / F_{2, \mathrm{~L}}$ vs. $Q$ from $\{u, d, s, c, b\}$ (green, blue, cyan, magenta, pink). (a) $F_{2}^{j} / F_{2}$ vs. $Q$. (b) $F_{\mathrm{L}}^{j} / F_{\mathrm{L}}$ vs. $Q$.

In figures 6 (a) and 6 (b), we display the fractional contributions for the initial-state quarks $(i)$ to the structure functions $F_{2}$ and $F_{\mathrm{L}}$, respectively, for selected $x$ values as a function of $Q$; here we have used $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{g, u, d, s, c, b\}$. We observe that for large $x$ and low $Q$ the heavy flavor contributions are minimal. For example, for $x=10^{-1}$ we see the contribution of the $u$ quark comprises $\sim 80 \%$ of the $F_{2}$ structure function at low $Q$. In contrast, at $x=10^{-5}$ and large $Q$, we see the $F_{2}$ contributions of the $u$ quark and $c$ quark are comparable (as they both couple with a factor $4 / 9$ ), and the $d$ quark and $s$ quark are comparable (as they both couple with a factor $1 / 9$ ). It is notable that the gluon contribution to $F_{\mathrm{L}}$ is significant. For $x=10^{-1}$ this is roughly $40 \%$ throughout the $Q$ range, and can be even larger for smaller $x$ values.

In figures 7 (a) and 7 (b), we display the fractional contributions for the final-state quarks $(j)$ to the structure functions $F_{2}$ and $F_{\mathrm{L}}$, respectively, for selected $x$ values as a function of $Q$; here we have used $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{u, d, s, c, b\}$. Again, we observe that for large $x$ and low $Q$ the heavy flavor contributions are minimal, but these can grow quickly as we move to smaller $x$ and larger $Q$.


Fig. 6. Fractional flavor decomposition of "initial-state" $F_{2, \mathrm{~L}}^{i} / F_{2, \mathrm{~L}}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for $n=2$ scaling. Reading from the bottom, we plot the cumulative contributions to $F_{2, \mathrm{~L}}$ from $\{g, u, d, s, c, b\}$, (red, green, blue, cyan, magenta, pink). (a) $F_{2}^{i} / F_{2}$ vs. $Q$. (b) $F_{\mathrm{L}}^{i} / F_{\mathrm{L}}$ vs. $Q$.


Fig. 7. Fractional contribution for each quark flavor to $F_{2, \mathrm{~L}}^{j} / F_{2, \mathrm{~L}}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). Results are displayed for $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{u, d, s, c, b\}$ (green, blue, cyan, magenta, pink). (a) $F_{2}^{j} / F_{2} v s . Q$. (b) $F_{\mathrm{L}}^{j} / F_{\mathrm{L}} v s . Q$.

In figure $8(\mathrm{a})$, we display the results for $F_{2}$ vs. $Q$ computed at various orders. For large $x(c f . \quad x=0.1)$ we find the perturbative calculation is particularly stable; we see that the LO result is within $20 \%$ of the others at small $Q$, and within $5 \%$ at large $Q$. The NLO is within $2 \%$ at small $Q$, and indistinguishable from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ for $Q$ values above $\sim 10 \mathrm{GeV}$. The NNLO and $\mathrm{N}^{3} \mathrm{LO}$ results are essentially identical throughout the kinematic range. For smaller $x$ values $\left(10^{-3}, 10^{-5}\right)$, the contribution of the higher order terms increases. Here, the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ coincide for $Q$ values above $\sim 5 \mathrm{GeV}$, but the NLO result can differ by $\sim 5 \%$.


Fig. 8. $F_{2, \mathrm{~L}}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for $n=2$ scaling. (a) $F_{2}$ vs. $Q$. (b) $F_{\mathrm{L}}$ vs. $Q$.

In Figure $8(\mathrm{~b})$, we display the results for $F_{\mathrm{L}}$ vs. $Q$ computed at various orders. In contrast to $F_{2}$, we find the NLO corrections are large for $F_{\mathrm{L}}$; this is because the $\mathrm{LO} F_{\mathrm{L}}$ contribution (which violates the Callan-Gross relation) is suppressed by $\left(m^{2} / Q^{2}\right)$ compared to the dominant gluon contributions which enter at NLO. Consequently, we observe (as expected) that the LO result for $F_{\mathrm{L}}$ receives large contributions from the higher order terms. Essentially, the NLO is the first non-trivial order for $F_{\mathrm{L}}$, and the subsequent contributions then converge. For example, at large $x(c f . x=0.1)$ for $Q \sim 10 \mathrm{GeV}$ we find the NLO result yields $\sim 60$ to $80 \%$ of the total, the NNLO is a $\sim 20 \%$ correction, and the $\mathrm{N}^{3} \mathrm{LO}$ is a $\sim 10 \%$ correction. For lower $x$ values $\left(10^{-3}\right.$, $10^{-5}$ ), the convergence of the perturbative series improves, and the NLO results is within $\sim 10 \%$ of the $\mathrm{N}^{3} \mathrm{LO}$ result. Curiously, for $x=10^{-5}$ the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ roughly compensate each other so that the NLO and the $\mathrm{N}^{3} \mathrm{LO}$ match quite closely for $Q \geq 2 \mathrm{GeV}$.

While the calculation of $F_{\mathrm{L}}$ is certainly more challenging, examining Fig. 1 we see that for most of the relevant kinematic range probed by HERA the theoretical calculation is quite stable. For example, in the high $Q^{2}$ region where HERA is probing intermediate $x$ values $\left(x \sim 10^{-3}\right)$ the spread of the $\chi(n)$ scalings is small. The challenge arises in the low $Q$ region $(Q \sim 2 \mathrm{GeV})$, where the $x$ values are $\sim 10^{-4}$; in this region, there is some spread between the various curves at the lowest $x$ value $\left(\sim 10^{-5}\right)$, but for $x \sim 10^{-3}$ this is greatly reduced.

## 5. Conclusions

We extended the ACOT calculation for DIS structure functions to $\mathrm{N}^{3} \mathrm{LO}$ by combining the exact ACOT scheme at NLO with a $\chi(n)$-rescaling which allows us to include the leading mass dependence at NNLO and $\mathrm{N}^{3} \mathrm{LO}$. Using the full ACOT calculation at NLO, we demonstrated that the heavy quarks mass dependence for the DIS structure functions is dominated by the kinematic mass contributions, and this can be implemented via a generalized $\chi(n)$-rescaling prescription.

We studied the $F_{2}$ and $F_{\mathrm{L}}$ structure functions as a function of $x$ and $Q$. We examined the flavor decomposition of these structure functions, and verified that the heavy quarks were appropriately suppressed in the low $Q$ region. We found the results for $F_{2}$ were very stable across the full kinematic range for $\{x, Q\}$, and the contributions from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ terms were small. For $F_{\mathrm{L}}$, the higher order terms gave a proportionally larger contribution (due to the suppression of the LO term from the Callan-Gross relation); nevertheless, the contributions from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ terms were generally small in the region probed by HERA.

The result of this calculation was to obtain precise predictions for the inclusive $F_{2}$ and $F_{\mathrm{L}}$ structure functions which can be used to analyze the HERA data.

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#### Abstract

We compute the structure functions $F_{2}$ and $F_{L}$ in the ACOT scheme for heavy quark production. We use the complete ACOT results to NLO, and make use of the $\overline{M S}$ massless results at NNLO and $\mathrm{N}^{3} \mathrm{LO}$ to estimate the higher order mass-dependent corrections. We show numerically that the dominant heavy quark mass effects can be taken into account using massless Wilson coefficients together with an appropriate rescaling prescription. Combining the exact NLO ACOT scheme with these expressions should provide a good approximation to the full calculation in the ACOT scheme at NNLO and $\mathrm{N}^{3} \mathrm{LO}$.


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## 1. Introduction

The production of heavy quarks in high energy processes has become an increasingly important subject of study both theoretically and experimentally. The theory of heavy quark production in perturbative Quantum Chromodynamics (pQCD) is more challenging than that of light parton (jet) production because of the new physics issues brought about by the additional heavy quark mass scale. The correct theory must properly take into account the changing role of the heavy quark over the full kinematic range of the relevant process from the threshold region (where the quark behaves like a typical "heavy particle") to the asymptotic region (where the

[^172]same quark behaves effectively like a parton, similar to the well known light quarks $\{u, d, s\}$ ).

With the ever-increasing precision of experimental data and the progression of theoretical calculations and parton distribution function (PDF) evolution to next-to-next-to-leading order (NNLO) of QCD there is a clear need to formulate and also implement the heavy quark schemes at this order and beyond. The most important case is arguably the heavy quark treatment in inclusive deep-inelastic scattering (DIS) since the very precise HERA data for DIS structure functions and cross sections form the backbone of any modern global analysis of PDFs. Here, the heavy quarks contribute up to $30 \%$ or $40 \%$ to the structure functions at small momentum fractions $x$. Extending the heavy quark schemes to higher orders is therefore necessary for extracting precise PDFs, and this is a prerequisite for precise predictions of observables at the LHC. However, we would like to also stress the theoretical importance of having a general pQCD framework that includes heavy quarks and is valid to all orders in perturbation theory over a wide range of hard energy scales.

An example, where higher order corrections are particularly important is the structure function $F_{L}$ in DIS. The leading order $\left(\mathcal{O}\left(\alpha_{S}^{0}\right)\right)$ contribution to this structure function vanishes for massless quarks due to helicity conservation (Callan-Gross relation). This has several consequences: 1) $F_{L}$ is useful for constraining the gluon PDF via the dominant subprocess $\gamma^{*} g \rightarrow q \bar{q}$. 2) The heavy quark mass effects of order $\mathcal{O}\left(\frac{m^{2}}{Q^{2}}\right)$ are relatively more pronounced 3) Since the first non-vanishing contribution to $F_{L}$ is next-to-leading order (up to mass effects), the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ corrections are more important than for $F_{2}$. In Fig. ⿴囗 we show a comparison of different theoretical calculations of $F_{L}$ with preliminary HERA data [2]. As can be seen, in particular at small $Q^{2}$ (i.e. small $x$ ), there are considerable differences between the predictions.

The purpose of this paper is to calculate the leading twist neutral current DIS structure functions $F_{2}$ and $F_{L}$ in the ACOT factorization scheme up to order $\mathcal{O}\left(\alpha_{S}^{3}\right)\left(\mathrm{N}^{3} \mathrm{LO}\right)$ and to estimate the error due to approximating the heavy quark mass terms $\mathcal{O}\left(\alpha_{S}^{2} \times \frac{m^{2}}{Q^{2}}\right)$ and $\mathcal{O}\left(\alpha_{S}^{3} \times \frac{m^{2}}{Q^{2}}\right)$ in the higher order corrections. The results of this study form the basis for using the ACOT scheme in NNLO global analyses and for future comparisons with precision data for DIS structure functions.

This paper is organized as follows. In Sec. 2 we review theoretical approaches to include heavy flavors in QCD calculations. Particular emphasis

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Fig. 1: $F_{L}$ vs. $Q$ from combined HERA-I inclusive deep inelastic cross sections measured by the H1 and ZEUS collaborations. Figure taken from Ref. [2].
is put on the ACOT scheme which is a minimal extension of the $\overline{M S}$ scheme. In Sec. 3 we present the prescription for constructing the approximate DIS structure functions in the ACOT scheme up to $\mathcal{O}\left(\alpha_{S}^{3}\right)$ order. The corresponding numerical results are presented in Sec. 4. Finally, in Sec. 5 we summarize the main results. This work is based on Ref. [3], and further details can be found therein.

## 2. Review of Theoretical Methods

We review theoretical methods which have been advanced to improve existing QCD calculations of heavy quark production, and the impact on recent experimental results.

### 2.1. ACOT Scheme

The ACOT renormalization scheme [4, 5] provides a mechanism to incorporate the heavy quark mass into the theoretical calculation of heavy quark production both kinematically and dynamically. In 1998 Collins [6] extended the factorization theorem to address the case of heavy quarks; this work provided the theoretical foundation that allows us to reliably compute heavy quark processes throughout the full kinematic realm.

If we consider the DIS production of heavy quarks at $\mathcal{O}\left(\alpha_{S}^{1}\right)$ this involves the $\mathrm{LO} Q V \rightarrow Q$ process and the NLO $g V \rightarrow Q \bar{Q}$ process ${ }^{2}$ The key ingredient provided by the ACOT scheme is the subtraction term (SUB)

[^174]which removes the "double counting" arising from the regions of phase space where the LO and NLO contributions overlap. Specifically, at NLO order, we can express the total result as a sum of
\[

$$
\begin{equation*}
\sigma_{T O T}=\sigma_{L O}+\left\{\sigma_{N L O}-\sigma_{S U B}\right\} \tag{1}
\end{equation*}
$$

\]

where the subtraction term for the gluon-initiated processes is

$$
\begin{equation*}
\sigma_{S U B}=f_{g} \otimes \tilde{P}_{g \rightarrow Q} \otimes \sigma_{Q V \rightarrow Q} . \tag{2}
\end{equation*}
$$

$\sigma_{S U B}$ represents a gluon emitted from a proton $\left(f_{g}\right)$ which undergoes a collinear splitting to a heavy quark ( $\tilde{P}_{g \rightarrow Q}$ ) convoluted with the LO quarkboson scattering $\sigma_{Q V \rightarrow Q}$. Here, $\tilde{P}_{g \rightarrow Q}(x, \mu)=\frac{\alpha_{s}}{2 \pi} \ln \left(\mu^{2} / m^{2}\right) P_{g \rightarrow Q}(x)$ where $P_{g \rightarrow Q}(x)$ is the usual $\overline{M S}$ splitting kernel, $m$ is the quark mass and $\mu$ is the renormalization scale which we typically choose to be $\mu=Q$.

An important feature of the ACOT scheme is that it reduces to the appropriate limit both as $m \rightarrow 0$ and $m \rightarrow \infty$ as we illustrate below. Specifically, in the limit where the quark $Q$ is relatively heavy compared to the characteristic energy scale ( $\mu \lesssim m$ ), we find $\sigma_{L O} \sim \sigma_{S U B}$ such that $\sigma_{T O T} \sim \sigma_{N L O}$. In this limit, the ACOT result naturally reduces to the Fixed-Flavor-Number-Scheme (FFNS) result. In the FFNS, the heavy quark is treated as being extrinsic to the hadron, and there is no corresponding heavy quark $\operatorname{PDF}\left(f_{Q} \sim 0\right)$; thus $\sigma_{L O} \sim 0$. We also have $\sigma_{S U B} \sim 0$ because this is proportional to $\ln \left(\mu^{2} / m^{2}\right)$. Thus, when the quark $Q$ is heavy relative to the characteristic energy scale $\mu$, the ACOT result reduces to $\sigma_{T O T} \sim \sigma_{N L O}$.

Conversely, in the limit where the quark $Q$ is relatively light compared to the characteristic energy scale $\left(\mu \gtrsim m\right.$ ), we find that $\sigma_{L O}$ yields the dominant part of the result, and the "formal" $\mathrm{NLO} \mathcal{O}\left(\alpha_{S}\right)$ contribution $\left\{\sigma_{N L O}-\sigma_{S U B}\right\}$ is an $\mathcal{O}\left(\alpha_{S}\right)$ correction. In this limit, the ACOT result will reduce to the $\overline{M S}$ Zero-Mass Variable-Flavor-Number-Scheme (ZMVFNS) limit exactly without any finite renormalizations. The quark mass $m$ no longer plays any dynamical role and purely serves as a regulator. The $\sigma_{N L O}$ term diverges due to the internal exchange of the quark $Q$, and this singularity is canceled by $\sigma_{S U B}$.

We illustrate the versatile role of the quark mass in Fig. 2a where we display $F_{2}^{c}$ as a function of $Q$ calculated in the ZM-VFNS, FFNS, ACOT, and S-ACOT schemes. We see that the ACOT scheme coincides with the FFNS for small $Q$, and the ZM-VFNS for large $Q$. In Fig. 2b we plot $F_{2}^{c}$ as a function of the quark mass $m$ for a fixed $Q=10 \mathrm{GeV}$ for the $\overline{M S}$ ZM-VFNS and ACOT schemes. We observe that when $m$ is within a decade or two of $\mu$, the quark mass plays a dynamic role; however, for $m \ll \mu$, the quark mass purely serves as a regulator and the specific value is not important.


Fig. 2: a) $F_{2}^{c}$ for $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number Scheme (FFNS), and Zero-Mass Variable Flavor Number Scheme (ZM-VFNS). The ACOT and S-ACOT results are virtually identical.
b) Comparison of $F_{2}^{c}(x, Q)$ (scaled by $10^{4}$ ) vs. the quark mass $m$ in GeV for fixed $x=0.1$ and $Q=10 \mathrm{GeV}$. The red dots are the full ACOT result, and the blue line is the massless $\overline{M S}$ result.

Operationally, it means we can obtain the $\overline{M S}$ ZM-VFNS result either by i) computing the terms using dimensional regularization and setting the regulator to zero, or ii) by computing the terms using the quark mass as the regulator and then setting this to zero.

The ACOT scheme is minimal in the sense that the construction of the massive short distance cross sections does not need any observabledependent extra contributions or any regulators to smooth the transition between the high and low scale regions. The ACOT prescription is: a) calculate the massive partonic cross sections, and b) perform the factorization using the quark mass as regulator.

It is in this sense that we claim the ACOT scheme is the minimal massive extension of the $\overline{M S}$ ZM-VFNS. In the limit $m / \mu \rightarrow 0$ it reduces exactly to the $\overline{M S}$ ZM-VFNS, in the limit $m / \mu \gtrsim 1$ the heavy quark decouples from the PDFs and we obtain exactly the FFNS for $m / \mu \gg 1$ and no finite renormalizations are needed.

## 2.2. $S$-ACOT

In a corresponding application, it was observed that the heavy quark mass could be set to zero in certain pieces of the hard scattering terms without any loss of accuracy. This modification of the ACOT scheme goes by the name Simplified-ACOT (S-ACOT) and can be summarized as follows [8].

S-ACOT: For hard-scattering processes with incoming heavy
quarks or with internal on-shell cuts on a heavy quark line, the heavy quark mass can be set to zero $(m=0)$ for these pieces.

If we consider the case of NLO DIS heavy quark production, this means we can set $m=0$ for the LO terms $\sigma_{Q V \rightarrow Q}$ (incoming heavy quark), and for the SUB terms (on-shell cut on an internal heavy quark line). Hence, the only contribution which requires calculation with $m$ retained is the NLO $g V \rightarrow Q \bar{Q}$ process. Figure 2a displays a comparison of a calculation using the ACOT scheme with all masses retained vs. the S-ACOT scheme; as expected, these two results match throughout the full kinematic region.

It is important to note that the S-ACOT scheme is not an approximation; this is an exact renormalization scheme, extensible to all orders.

### 2.3. ACOT and $\chi$-Rescaling

As we have illustrated in Sec. 2.1, in the limit $Q^{2} \gg m^{2}$ the mass simply plays the role of a regulator. In contrast, for $Q^{2} \sim m^{2}$ the value of the mass is of consequence for the physics. The mass can enter dynamically in the hard-scattering matrix element, and can enter kinematically in the phase space of the process.

We will demonstrate that for the processes of interest the primary role of the mass is kinematic and not dynamic. It was this idea which was behind the original slow-rescaling prescription of [9] which considered DIS charm production (e.g., $\gamma c \rightarrow c$ ) introducing the shift $x \rightarrow \chi=x\left[1+\left(m_{c} / Q\right)^{2}\right]$. This prescription accounted for the charm quark mass by effectively reducing the phase space for the final state by an amount proportional to $\left(m_{c} / Q\right)^{2}$.

This idea was extended in the $\chi$-scheme by realizing that (in most cases) in addition to the observed final-state charm quark, there is also an anticharm quark in the beam fragments since all the charm quarks are ultimately produced by gluon splitting $(g \rightarrow c \bar{c})$ into a charm pair. For this case the scaling variable becomes $\chi=x\left[1+\left(2 m_{c} / Q\right)^{2}\right]$. This rescaling is implemented in the $\mathrm{ACOT}_{\chi}$ scheme, for example [10-12] $]^{3}$ The factor $\left(1+\left(2 m_{c}\right)^{2} / Q^{2}\right)$ represents a kinematic suppression factor which will suppress the charm process relative to the lighter quarks. Additionally, the $\chi$-scaling ensures the threshold kinematics $\left(W^{2}>4 m^{2}+M^{2}\right)$ is satisfied; while it is important to satisfy this condition for large $x$, this may prove too restrictive at small $x$ where the HERA data are especially precise.

To encompass all the above results, we can define a general scaling variable $\chi(n)$ as

$$
\begin{equation*}
\chi(n)=x\left[1+\left(\frac{n m_{c}}{Q}\right)^{2}\right] \tag{3}
\end{equation*}
$$

[^175]
(a) Comparison of $F_{2}^{c}(x, Q)$ vs. $Q$ for the NLO ACOT calculation for $x=$ $\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) using zero dynamic mass $[\widehat{\sigma}(m=0)]$ to show the effect of $n$ scaling; from top to bottom $n=\{0,1,2\}$ (pink, black, purple).

(b) Comparison of $F_{2}^{c}(x, Q)$ vs. $Q$ for the NLO ACOT calculation for $x=$ $\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). Here we keep the scaling fixed $n=2$ and compare the effect of varying the dynamic mass in the Wilson coefficient. The upper (cyan) curve uses a non-zero dynamic mass $[\widehat{\sigma}(m=1.3)]$ and the lower (purple) curve uses a zero dynamic mass $[\widehat{\sigma}(m=0)]$.
Fig. 3: Comparison of Phase Space (Kinematic) \& Dynamic Mass Effects
where $n=\{0,1,2\}$. Here, $n=0$ corresponds to the massless result without rescaling, $n=1$ corresponds to the original Barnett slow-rescaling, and $n=2$ corresponds to the $\chi$-rescaling.

### 2.4. Phase Space (Kinematic) \& Dynamic Mass

We now investigate the effects of separately varying the mass entering the $\chi(n)$ variable taking into account the phase space constraints and the mass value entering the hard scattering cross section $\widehat{\sigma}(m)$. We call the former mass parameter "phase space (kinematic) mass" and the latter "dynamic mass".

In Fig. 3a we display $F_{2}^{c}(x, Q)$ vs. $Q$. The family of 3 curves shows the NLO ACOT calculation with $\chi(n)$ scaling using a zero dynamic mass for the hard scattering. We compare this with Fig. 3b which shows $F_{2}^{c}(x, Q)$ in the NLO ACOT scheme using a fixed $n=2$ scaling, but varying the mass used in the hard-scattering cross section. The upper (cyan) curves use a non-zero dynamic mass $\left[\widehat{\sigma}\left(m_{c}=1.3\right)\right]$ and the lower (purple) curves have been obtained with a vanishing dynamic mass $\left[\widehat{\sigma}\left(m_{c}=0\right)\right]$. We observe that the effect of the 'dynamic mass' in $\widehat{\sigma}\left(m_{c}\right)$ is only of consequence in
the limited region $Q \gtrsim m$, and even in this region the effect is minimal. In contrast, the influence of the phase space (kinematic) mass shown in Fig. 3a is larger than the dynamic mass shown in Fig. 3b,

In conclusion, we have shown that (up to $\mathcal{O}\left(\alpha_{S}\right)$ ) the phase space mass dependence is generally the dominant contribution to the DIS structure functions. Assuming that this observation remains true at higher orders, it is possible to obtain a good approximation of the structure functions in the ACOT scheme at NNLO and $\mathrm{N}^{3} \mathrm{LO}$ using the massless Wilson coefficients together with a non-zero phase space mass entering via the $\chi(n)$ prescription.

### 2.5. Other massive schemes

There are a number of other schemes for incorporating the heavy quark mass terms, and we briefly note a few examples. The Thorne-Roberts (TR) scheme [14, 15] and its derivatives (TR') are designed to provide a smooth threshold behavior, and this is implemented by including pieces of the higher order contributions. The FONLL scheme [16] was originally developed to match fixed order calculations with resumed ones in the case of heavy quark hadroproduction; this approach has been generalized and applied to other applications including DIS structure functions [17]. Details and comparisons of these approached is outlined in the 2009 Les Houches Workshop report [18].

## 3. ACOT scheme beyond NLO

In Sec. 2.4 we have shown using the NLO full ACOT scheme that the dominant mass effects are those coming from the phase space which can be taken into account via a generalized slow-rescaling $\chi(n)$-prescription. Assuming that a similar relation remains true at higher orders one can construct the following approximation to the full ACOT result up to $\mathrm{N}^{3} \mathrm{LO}$ $\left(\mathcal{O}\left(\alpha_{S}^{3}\right)\right)$ :

$$
\begin{equation*}
\operatorname{ACOT}\left[\mathcal{O}\left(\alpha_{S}^{0+1+2+3}\right)\right] \simeq \operatorname{ACOT}\left[\mathcal{O}\left(\alpha_{S}^{0+1}\right)\right]+{\mathrm{ZM}-\operatorname{VFNS}_{\chi}\left[\mathcal{O}\left(\alpha_{S}^{2+3}\right)\right] . . . ~}_{\text {. }} \tag{4}
\end{equation*}
$$

Here, the massless Wilson coefficients at $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$ and $\mathcal{O}\left(\alpha \alpha_{S}^{3}\right)$ are substituted for the Wilson coefficients in the ACOT scheme as the corresponding massive coefficients have not yet been computed.

There has been a calculation of neutral current electroproduction (equal quark masses, vector coupling) of heavy quarks at this order by Smith \& VanNeerven [19] in the FFNS which could be used to obtain the massive Wilson coefficients in the S-ACOT scheme by applying appropriate collinear
subtraction terms $\sqrt{4}^{4}$ however, this is beyond the scope of this paper. For charge current case massive calculations are available at order $\mathcal{O}\left(\alpha \alpha_{S}\right)$ [21]23] and partial results at order $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$ [24.

Here, we argue that the massless Wilson coefficients at $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$ together with a $\chi(n)$-prescription provide a very good approximation of the exact result. At worst, the maximum error would be of order $\mathcal{O}\left(\alpha \alpha_{S}^{2} \times\left[m^{2} / Q^{2}\right]\right)$. However, based on the arguments of Sec. 2.4 we expect the inclusion of the phase space mass effects to contain the dominant higher order contributions so that the actual error should be substantially smaller.

The massless higher order coefficient functions for the DIS structure function $F_{2}$ via photon exchange can be found in Refs. 25$] 34$. The expressions for the structure function $F_{L}$ have been calculated in Refs. [29, 31, 33, (35, 36.

We now consider our choice for the appropriate generalized $\chi(n)$-rescaling variable. For the purposes of this study, we will vary the phase space mass using the $\chi(n)$ rescaling with $n=\{0,1,2\}$. While $n=0$ corresponds to the massless case (no rescaling), it is not obvious whether $n=1$ or $n=2$ is the preferred rescaling choice for higher orders. Thus, we will use the range between $n=1$ and $n=2$ as a measure of our theoretical uncertainty arising from this ambiguity.

## 4. Results

We now present our results for the $F_{2}$ and $F_{L}$ structure functions calculated at $\mathrm{N}^{3} \mathrm{LO}$ in the extended ACOT scheme. The initial PDFs, based on the Les Houches benchmark set [37] are evolved using the QCDNUM program [38]. In the calculation we set $m_{c}=1.3 \mathrm{GeV}, m_{b}=4.5 \mathrm{GeV}$ and $\alpha_{s}\left(M_{Z}\right)=0.118$.

In Figures 4a and 4b we display the structure functions $F_{2}$ and $F_{L}$, respectively, for selected $x$ values as a function of $Q$. Each plot has three curves which are computed using $n$-scalings of $\{0,1,2\}$. We observe that the effect of the $n$-scaling is negligible except for very small $Q$ values. This result is in part because the heavy quarks are only a fraction of the total structure function, and the effects of the $n$-scaling are reduced at larger $Q$ values.

In Ref. [3] we magnify the small $Q$ region of $F_{L}$ of Fig. 4b for $x=10^{-5}$, where the effects of using different scalings are largest. We can see that for inclusive observables, the $n=1$ and $n=2$ scalings give nearly identical results, but they differ from the massless case $(n=0)$. This result, together

[^176]

Fig. 4: $F_{2, L}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). The three lines show the scaling variable: $n=\{0,1,2\}$ (red, green, blue). We observe the effect of the $n$-scaling is negligible except for very small $Q$ values.
with the observation that at NLO kinematic mass effects are dominant, suggests that the error we have in our approach is relatively small and approximated by the band between $n=1$ and $n=2$ results.

We can investigate the effects of the $\chi(n)$-scaling in more details by examining the flavor decomposition of the structure functions. In Figures 5 a and 5b we display the fractional contributions of quark flavors to the structure functions $F_{2, L}$ for selected $n$-scaling values as a function of $Q$. We observe the $n$-scaling reduces the relative contributions of charm and bottom at low $Q$ scales. For example, without any $n$-scaling $(n=0)$ we find the charm and bottom quarks contribute an unusually large fraction at very low scales $\left(Q \sim m_{c}\right)$ as they are (incorrectly) treated as massless partons in this region. The result of the different $n$-scalings $(n=1,2)$ is to introduce a kinematic penalty which properly suppresses the contribution of these heavy quarks in the low $Q$ region. In the following, we will generally use the $n=2$ scaling for our comparisons.

In Figures 6a and 6b we display the fractional contributions for the initial-state quarks $(i)$ to the structure functions $F_{2}$ and $F_{L}$, respectively, for selected $x$ values as a function of $Q$; here we have used $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{g, u, d, s, c, b\}$. We observe that for large $x$ and low $Q$ the heavy flavor contributions are minimal. For example, for $x=10^{-1}$ we see the contribution


Fig. 5: Effect of $\chi(n)$-scaling for $n=\{0,1,2\}$ (left to right) at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-3}\right\}$. Reading from the bottom we have fractional contribution for each (final-state) quark flavor to $F_{2, L}^{j} / F_{2, L}$ vs. $Q$ from $\{u, d, s, c, b\}$ (green, blue, cyan, magenta, pink).


Fig. 6: Fractional flavor decomposition of "initial-state" $F_{2, L}^{i} / F_{2, L}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for $n=2$ scaling. Reading from the bottom, we plot the cumulative contributions to $F_{2, L}$ from $\{g, u, d, s, c, b\}$, (red, green, blue, cyan, magenta, pink).


Fig. 7: Fractional contribution for each quark flavor to $F_{2, L}^{j} / F_{2, L}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). Results are displayed for $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{u, d, s, c, b\}$ (green, blue, cyan, magenta, pink).
of the $u$-quark comprises $\sim 80 \%$ of the $F_{2}$ structure function at low $Q$. In contrast, at $x=10^{-5}$ and large $Q$ we see the $F_{2}$ contributions of the $u$ quark and $c$-quark are comparable (as they both couple with a factor $4 / 9$ ), and the $d$-quark and $s$-quark are comparable (as they both couple with a factor $1 / 9$ ). It is notable that the gluon contribution to $F_{L}$ is significant. For $x=10^{-1}$ this is roughly $40 \%$ throughout the $Q$ range, and can be even larger for smaller $x$ values.

In Figures 7a and 7b we display the fractional contributions for the final-state quarks $(j)$ to the structure functions $F_{2}$ and $F_{L}$, respectively, for selected $x$ values as a function of $Q$; here we have used $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{u, d, s, c, b\}$. Again, we observe that for large $x$ and low $Q$ the heavy flavor contributions are minimal, but these can grow quickly as we move to smaller $x$ and larger $Q$.

In Figure we display the results for $F_{2}$ vs. $Q$ computed at various orders. For large $x$ (c.f. $x=0.1$ ) we find the perturbative calculation is particularly stable; we see that the LO result is within $20 \%$ of the others at small $Q$, and within $5 \%$ at large $Q$. The NLO is within $2 \%$ at small $Q$, and indistinguishable from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ for $Q$ values above $\sim 10 \mathrm{GeV}$. The NNLO and $\mathrm{N}^{3} \mathrm{LO}$ results are essentially identical throughout the kinematic range. For smaller $x$ values $\left(10^{-3}, 10^{-5}\right)$ the contribution of


Fig. 8: $F_{2, L}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for $n=2$ scaling.
the higher order terms increases. Here, the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ coincide for $Q$ values above $\sim 5 \mathrm{GeV}$, but the NLO result can differ by $\sim 5 \%$.

In Figure 8 b we display the results for $F_{L}$ vs. $Q$ computed at various orders. In contrast to $F_{2}$, we find the NLO corrections are large for $F_{L}$; this is because the LO $F_{L}$ contribution (which violates the Callan-Gross relation) is suppressed by $\left(m^{2} / Q^{2}\right)$ compared to the dominant gluon contributions which enter at NLO. Consequently, we observe (as expected) that the LO result for $F_{L}$ receives large contributions from the higher order terms. Essentially, the NLO is the first non-trivial order for $F_{L}$, and the subsequent contributions then converge. For example, at large $x$ (c.f. $x=0.1$ ) for $Q \sim 10 \mathrm{GeV}$ we find the NLO result yields $\sim 60$ to $80 \%$ of the total, the NNLO is a $\sim 20 \%$ correction, and the $\mathrm{N}^{3} \mathrm{LO}$ is a $\sim 10 \%$ correction. For lower $x$ values $\left(10^{-3}, 10^{-5}\right)$ the convergence of the perturbative series improves, and the NLO results is within $\sim 10 \%$ of the $\mathrm{N}^{3} \mathrm{LO}$ result. Curiously, for $x=10^{-5}$ the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ roughly compensate each other so that the NLO and the $\mathrm{N}^{3} \mathrm{LO}$ match quite closely for $Q \geq 2 \mathrm{GeV}$.

While the calculation of $F_{L}$ is certainly more challenging, examining Fig. Tiwe see that for most of the relevant kinematic range probed by HERA the theoretical calculation is quite stable. For example, in the high $Q^{2}$ region where HERA is probing intermediate $x$ values $\left(x \sim 10^{-3}\right)$ the spread of the $\chi(n)$ scalings is small. The challenge arises in the low $Q$ region ( $Q \sim 2 \mathrm{GeV}$ ) where the $x$ values are $\sim 10^{-4}$; in this region, there is some spread between the various curves at the lowest $x$ value $\left(\sim 10^{-5}\right)$, but for $x \sim 10^{-3}$ this is
greatly reduced.

## 5. Conclusions

We extended the ACOT calculation for DIS structure functions to $\mathrm{N}^{3} \mathrm{LO}$ by combining the exact ACOT scheme at NLO with a $\chi(n)$-rescaling which allows us to include the leading mass dependence at NNLO and $\mathrm{N}^{3} \mathrm{LO}$. Using the full ACOT calculation at NLO, we demonstrated that the heavy quarks mass dependence for the DIS structure functions is dominated by the kinematic mass contributions, and this can be implemented via a generalized $\chi(n)$-rescaling prescription.

We studied the $F_{2}$ and $F_{L}$ structure functions as a function of $x$ and $Q$. We examined the flavor decomposition of these structure functions, and verified that the heavy quarks were appropriately suppressed in the low $Q$ region. We found the results for $F_{2}$ were very stable across the full kinematic range for $\{x, Q\}$, and the contributions from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ terms were small. For $F_{L}$, the higher order terms gave a proportionally larger contribution (due to the suppression of the LO term from the Callan-Gross relation); nevertheless, the contributions from the NNLO and $\mathrm{N}^{3}$ LO terms were generally small in the region probed by HERA.

The result of this calculation was to obtain precise predictions for the inclusive $F_{2}$ and $F_{L}$ structure functions which can be used to analyze the HERA data.

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# Heavy quark production in the Aivazis-Collins-Olness-Tung scheme at next-to-next-to-leading and next-to-next-to-next-to-leading order 

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#### Abstract

We analyze the properties of the Aivazis-Collins-Olness-Tung (ACOT) scheme for heavy quark production and make use of the $\overline{\mathrm{MS}}$ massless results at next-to-next-to-leading order and $\mathrm{N}^{3} \mathrm{LO}$ for the structure functions $F_{2}$ and $F_{L}$ in neutral current deep-inelastic scattering to estimate the higher order corrections. For this purpose we decouple the heavy quark mass entering the phase space from the one entering the dynamics of the short distance cross section. We show numerically that the phase space mass is generally more important. Therefore, the dominant heavy quark mass effects at higher orders can be taken into account using the massless Wilson coefficients together with an appropriate slow-rescaling prescription implementing the phase space constraints. Combining the exact ACOT scheme at next-toleading order with these expressions should provide a good approximation to the missing full calculation in the ACOT scheme at next-to-next-to-leading order and $\mathrm{N}^{3} \mathrm{LO}$.


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## I. INTRODUCTION

## A. Motivation

The production of heavy quarks in high energy processes has become an increasingly important subject of study both theoretically and experimentally. The theory of heavy quark production in perturbative quantum chromodynamics is more challenging than that of light parton (jet) production because of the new physics issues brought about by the additional heavy quark mass scale. The correct theory must properly take into account the changing role of the heavy quark over the full kinematic range of the relevant process from the threshold region (where the quark behaves like a typical "heavy particle") to the asymptotic region (where the same quark behaves effectively like a parton, similar to the well-known light quarks $\{u, d, s\}$ ).

With the ever-increasing precision of experimental data and the progression of theoretical calculations and parton distribution function (PDF) evolution to next-to-next-toleading order (NNLO) of QCD there is a clear need to formulate and also implement the heavy quark schemes at this order and beyond. The most important case is arguably the heavy quark treatment in inclusive deep-inelastic scattering (DIS) since the very precise HERA data for DIS structure functions and cross sections form the backbone of

[^177]any modern global analysis of PDFs. Here, the heavy quarks contribute up to $30 \%$ or $40 \%$ to the structure functions at small momentum fractions $x$. Extending the heavy quark schemes to higher orders is therefore necessary for extracting precise PDFs and hence for precise predictions of observables at the LHC. However, we would like to also stress the theoretical importance of having a general perturbative quantum chromodynamic framework including heavy quarks which is valid to all orders in perturbation theory over a wide range of hard energy scales and which is also applicable to other observables than inclusive DIS in a straightforward manner.

An example, where higher order corrections are particularly important is the structure function $F_{L}$ in DIS. The leading $\operatorname{order}\left(\mathcal{O}\left(\alpha_{S}^{0}\right)\right)$ contribution to this structure function vanishes for massless quarks due to helicity conservation (Callan-Gross relation). This has several consequences:
(i) $F_{L}$ is useful for constraining the gluon PDF via the dominant subprocess $\gamma^{*} g \rightarrow q \bar{q}$.
(ii) The heavy quark mass effects of order $\mathcal{O}\left(\frac{m^{2}}{Q^{2}}\right)$ are relatively more pronounced. ${ }^{1}$
(iii) Since the first nonvanishing contribution to $F_{L}$ is next-to-leading order (up to mass effects), the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ corrections are more important than for $F_{2}$.

In Fig. 1 we show a comparison of different theoretical calculations of $F_{L}$ with preliminary HERA data [2]. As can

[^178]

FIG. 1 (color online). $\quad F_{L}$ vs $Q$ from combined HERA-I inclusive deep inelastic cross sections measured by the H1 and ZEUS collaborations. Figure taken from Ref. [2].
be seen, in particular, at small $Q^{2}$ (i.e. small $x$ ), there are considerable differences between the predictions. ${ }^{2}$

The purpose of this paper is to calculate the leading twist neutral current DIS structure functions $F_{2}$ and $F_{L}$ in the Aivazis-Collins-Olness-Tung (ACOT) factorization scheme up to order $\mathcal{O}\left(\alpha_{S}^{3}\right)\left(\mathrm{N}^{3} \mathrm{LO}\right)$ and to estimate the error due to approximating the heavy quark mass terms $\mathcal{O}\left(\alpha_{S}^{2} \times \frac{m^{2}}{Q^{2}}\right)$ and $\mathcal{O}\left(\alpha_{S}^{3} \times \frac{m^{2}}{Q^{2}}\right)$ in the higher order corrections. The results of this study form the basis for using the ACOT scheme in NNLO global analyses and for future comparisons with precision data for DIS structure functions.

## B. Outline of paper

The rest of this paper is organized as follows. In Sec. II we review theoretical approaches to include heavy flavors in QCD calculations. Particular emphasis is put on the ACOT scheme which is the minimal extension of the $\overline{\mathrm{MS}}$ scheme in the sense that the observables in the ACOT scheme reduce to the ones in the $\overline{\mathrm{MS}}$ scheme in the limit $m \rightarrow 0$ without any finite renormalizations. In this discussion we explicitly distinguish between the heavy quark/ heavy meson mass entering the final state phase space which we will call "phase space mass" and the heavy quark mass entering the dynamics of the short distance cross section denoted "dynamic mass." We show numerically using the exact ACOT scheme at $\mathcal{O}\left(\alpha_{S}\right)$ next-toleading order (NLO) that the effects of the phase space mass are more important than the ones due to the dynamic mass. We use this observation to construct in Sec. III the NC DIS structure functions in the ACOT scheme up to $\mathcal{O}\left(\alpha_{S}^{3}\right)$. The corresponding numerical results are presented in Sec. IV. Finally, in Sec. V we summarize the main results.

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FIG. 2 (color online). Characteristic Feynman graphs which contribute to DIS heavy quark production in the ACOT scheme: (a) the LO $\mathcal{O}\left(\alpha_{S}^{0}\right)$ quark-boson scattering $Q V \rightarrow Q$, (b) the NLO $\mathcal{O}\left(\alpha_{S}^{1}\right)$ gluon-boson scattering $g V \rightarrow Q \bar{Q}$, and (c) the corresponding subtraction term (SUB) $(g \rightarrow Q \bar{Q}) \otimes(Q \rightarrow g Q)$.

## II. REVIEW OF THEORETICAL METHODS

We review theoretical methods which have been advanced to improve existing QCD calculations of heavy quark production, and the impact on recent experimental results.

## A. ACOT scheme

The ACOT renormalization scheme [4] provides a mechanism to incorporate the heavy quark mass into the theoretical calculation of heavy quark production both kinematically and dynamically. In 1998 Collins [5] extended the factorization theorem to address the case of heavy quarks; this work provided the theoretical foundation that allows us to reliably compute heavy quark processes throughout the full kinematic realm.

Figure 2 displays characteristic Feynman graphs for the first two orders of DIS heavy quark production. If we consider the DIS production of heavy quarks at $\mathcal{O}\left(\alpha_{S}^{1}\right)$ this involves the leading order (LO) $Q V \rightarrow Q$ process and the NLO $g V \rightarrow Q \bar{Q}$ process. ${ }^{3}$

The key ingredient provided by the ACOT scheme is the subtraction term (SUB) which removes the "double counting" arising from the regions of phase space where the LO and NLO contributions overlap. Specifically, at NLO order, we can express the total result as a sum of

$$
\begin{equation*}
\sigma_{\mathrm{TOT}}=\sigma_{\mathrm{LO}}+\left\{\sigma_{\mathrm{NLO}}-\sigma_{\mathrm{SUB}}\right\} \tag{1}
\end{equation*}
$$

where the subtraction term for the gluon-initiated processes is

$$
\begin{equation*}
\sigma_{\mathrm{SUB}}=f_{g} \otimes \tilde{P}_{g \rightarrow Q} \otimes \sigma_{Q V \rightarrow Q} \tag{2}
\end{equation*}
$$

$\sigma_{\text {SUB }}$ represents a gluon emitted from a proton $\left(f_{g}\right)$ which undergoes a collinear splitting to a heavy quark $\left(\tilde{P}_{g \rightarrow Q}\right)$ convoluted with the LO quark-boson scattering $\sigma_{Q V \rightarrow Q}$. Here, $\tilde{P}_{g \rightarrow Q}(x, \mu)=\frac{\alpha_{s}}{2 \pi} \ln \left(\mu^{2} / m^{2}\right) P_{g \rightarrow Q}(x)$ where $P_{g \rightarrow Q}(x)$ is the usual $\overline{\mathrm{MS}}$ splitting kernel, $m$ is the quark

[^180]mass and $\mu$ is the renormalization scale ${ }^{4}$ which we typically choose to be $\mu=Q$.

An important feature of the ACOT scheme is that it reduces to the appropriate limit both as $m \rightarrow 0$ and $m \rightarrow \infty$ as we illustrate below.

## 1. Fixed-flavor-number-scheme limit

Specifically, in the limit where the quark $Q$ is relatively heavy compared to the characteristic energy scale ( $\mu \lesssim$ $m$ ), we find $\sigma_{\mathrm{LO}} \sim \sigma_{\mathrm{SUB}}$ such that $\sigma_{\mathrm{TOT}} \sim \sigma_{\mathrm{NLO}}$. In this limit, the ACOT result naturally reduces to the fixed-flavor-number-scheme (FFNS) result. In the FFNS, the heavy quark is treated as being extrinsic to the hadron, and there is no corresponding heavy quark $\operatorname{PDF}\left(f_{Q} \sim 0\right)$; thus $\sigma_{\mathrm{LO}} \sim 0$. We also have $\sigma_{\mathrm{SUB}} \sim 0$ because this is proportional to $\ln \left(\mu^{2} / m^{2}\right)$. Thus, when the quark $Q$ is heavy relative to the characteristic energy scale $\mu$, the ACOT result reduces to $\sigma_{\mathrm{TOT}} \sim \sigma_{\mathrm{NLO}}$.

## 2. Zero-mass variable-flavor-number-scheme limit

Conversely, in the limit where the quark $Q$ is relatively light compared to the characteristic energy scale ( $\mu \gtrsim m$ ), we find that $\sigma_{\text {LO }}$ yields the dominant part of the result, and the "formal" $\mathrm{NLO} \mathcal{O}\left(\alpha_{S}\right)$ contribution $\left\{\sigma_{\mathrm{NLO}}-\sigma_{\mathrm{SUB}}\right\}$ is an $\mathcal{O}\left(\alpha_{S}\right)$ correction.

In the limit $m / \mu \rightarrow 0$, the ACOT result will reduce to the $\overline{\mathrm{MS}}$ zero-mass variable-flavor-number-scheme (ZMVFNS) limit exactly without any finite renormalizations. In this limit, the quark mass $m$ no longer plays any dynamical role and purely serves as a regulator. The $\sigma_{\mathrm{NLO}}$ term diverges due to the internal exchange of the quark $Q$, and this singularity will be canceled by $\sigma_{\text {SUB }}$.

## 3. ACOT as a minimal extension of $\overline{\mathrm{MS}}$

We illustrate the versatile role of the quark mass in Fig. 3(a) where we display the $\overline{\mathrm{MS}} \mathrm{ZM}-V F N S$ and the ACOT result as a function of the quark mass $m$.

We observe that when $m$ is within a decade or two of $\mu$ that the quark mass plays a dynamic role; however, for $m \ll \mu$, the quark mass purely serves as a regulator and the specific value is not important. Operationally, it means we can obtain the $\overline{\mathrm{MS}}$ ZM-VFNS result either by i) computing the terms using dimensional regularization and setting the regulator to zero, or ii) by computing the terms using the quark mass as the regulator and then setting this to zero. ${ }^{5}$ To demonstrate this point explicitly, in Fig. 3(b) we again display the $\overline{\mathrm{MS}} \mathrm{ZM}-\mathrm{VFNS}$ and the ACOT results

[^181]

FIG. 3 (color online). Comparison of $F_{2}^{c}(x, Q)$ (scaled by $10^{4}$ ) vs the quark mass $m$ in GeV for fixed $x=0.1$ and $Q=10 \mathrm{GeV}$. The red dots are the full ACOT result, and the blue line is the massless $\overline{\mathrm{MS}}$ result. The logarithmic plot demonstrates this result holds precisely in the $m \rightarrow 0$ limit.
but this time with a logarithmic scale to highlight the small $m$ region. We clearly see that ACOT reduces the $\overline{\mathrm{MS}} \mathrm{ZM}-$ VFNS exactly in this limit without any additional finite renormalization contributions. ${ }^{6}$

The ACOT scheme is minimal in the sense that the construction of the massive short distance cross sections does not need any observable-dependent extra contributions or any regulators to smooth the transition between the high and low scale regions. The ACOT prescription is to just calculate the massive partonic cross sections and perform the factorization using the quark mass as regulator.

It is in this sense that we claim the ACOT scheme is the minimal massive extension of the $\overline{\mathrm{MS}}$ ZM-VFNS. In the limit $m / \mu \rightarrow 0$ it reduces exactly to the $\overline{\mathrm{MS}}$ ZM-VFNS, in the limit $m / \mu \gtrsim 1$ the heavy quark decouples from the PDFs and we obtain exactly the FFNS for $m / \mu \gg 1$ and no finite renormalizations or additional parameters are needed.

## 4. When do we need heavy quark PDFs

The novel ingredient in the above calculation is the inclusion of the heavy quark PDF contribution which

[^182]

FIG. 4. Comparison of the DGLAP evolved charm PDF $f_{c}(x, \mu)$ with the perturbatively computed single splitting (SUB) $\tilde{f}_{c}(x, \mu)=f_{g}(x, \mu) \otimes \tilde{P}_{g \rightarrow c}$ vs $\mu$ in GeV for two representative values of $x$.
resums logs of $\alpha_{S} \ln \left(\mu^{2} / m^{2}\right)$. An obvious question is when do we need to consider such terms, and how large are their contributions? The answer is illustrated in Fig. 4 where we compare the Dokshitzer, Gribov, Lipatov, Altarelli, Parisi (DGLAP) evolved PDF $f_{Q}(x, \mu)$ with the single splitting perturbative result $\tilde{f}_{Q}(x, \mu)$.

The DGLAP PDF evolution sums a nonperturbative infinite tower of logs which are contained in $\sigma_{\text {LO }}$ while the $\sigma_{\text {SUB }}$ contribution removes the perturbative single splitting component which is already included in the $\sigma_{\text {NLO }}$ contribution. Hence, at the PDF level the difference between the heavy quark DGLAP evolved PDF $f_{Q}$ and the single-splitting perturbative $\tilde{f}_{Q}$ will indicate the contribution of the higher order logs which are resummed into the heavy quark PDF. Here, $\tilde{f}_{Q}=f_{g} \otimes \tilde{P}_{g \rightarrow Q}$ represents the PDF of a heavy quark $Q$ generated from a single perturbative splitting.

For $\mu \sim m$ we see that $f_{Q}$ and $\tilde{f}_{Q}$ match quite closely, whereas they differ significantly for $\mu$ values a few times $m$. While the details will depend on the specific process, in general we find that for $\mu$-scales a few times $m$ the terms resummed by the heavy quark PDF can be significant. Additionally, the difference between $f_{Q}$ and $\tilde{f}_{Q}$ will be reduced at higher orders as more perturbative splittings are included in $\tilde{f}_{Q}$.

Note that these scales are much lower than one might estimate using the naive criterion $\frac{\alpha_{S}}{2 \pi} \ln \left(\mu^{2} / m^{2}\right) \sim 1$; in particular, the ACOT calculation often yields reduced $\mu$ dependence as the quark dominated $\sigma_{\text {LO }}$ contributions typically have behavior which is complementary to the gluon-initiated $\sigma_{\text {NLO }}$ terms.

## B. S-ACOT

In a corresponding application, it was observed that the heavy quark mass could be set to zero in certain pieces of the hard scattering terms without any loss of accuracy. This modification of the ACOT scheme goes by the name simplified-ACOT (S-ACOT) and can be summarized as follows [8].

S-ACOT: For hard-scattering processes with incoming heavy quarks or with internal on-shell cuts on a heavy quark line, the heavy quark mass can be set to zero $(m=0)$ for these pieces.

If we consider the case of NLO DIS heavy quark production, this means we can set $m=0$ for the LO terms $(Q V \rightarrow Q)$ as this involves an incoming heavy quark, and we can set $m=0$ for the SUB terms as this has an on-shell cut on an internal heavy quark line. Hence, the only contribution which requires calculation with $m$ retained is the NLO $g V \rightarrow Q \bar{Q}$ process. Figure 5 displays a comparison of a calculation using the ACOT scheme with all masses retained vs the S-ACOT scheme; as expected, these two results match throughout the full kinematic region.

It is important to note that the S-ACOT scheme is not an approximation; this is an exact renormalization scheme, extensible to all orders.

## C. ACOT and $\boldsymbol{\chi}$ rescaling

As we have illustrated in Sec. II A above, in the limit $Q^{2} \gg m^{2}$ the mass simply plays the role of a regulator. In contrast, for $Q^{2} \sim m^{2}$ the value of the mass is of consequence for the physics. The mass can enter dynamically


FIG. 5 (color online). $F_{2}^{c}$ for $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, FFNS, and ZM-VFNS. The ACOT and S-ACOT results are virtually identical.
in the hard-scattering matrix element, and can enter kinematically in the phase space of the process.

We will demonstrate that for the processes of interest the primary role of the mass is kinematic and not dynamic. It was this idea which was behind the original slow-rescaling prescription of [9] which considered DIS charm production (e.g., $\gamma c \rightarrow c$ ) introducing the shift

$$
\begin{equation*}
x \rightarrow \chi=x\left[1+\left(\frac{m_{c}}{Q}\right)^{2}\right] \tag{3}
\end{equation*}
$$

This prescription accounted for the charm quark mass by effectively reducing the phase space for the final state by an amount proportional to $\left(m_{c} / Q\right)^{2}$.

This idea was extended in the $\chi$-scheme by realizing that in addition to the observed final-state charm quark, if the beam has a charm-flavor quantum number of zero (such as a proton beam) then there is also an anticharm quark in the beam fragments because all the charm quarks are ultimately produced by gluon splitting ( $g \rightarrow c \bar{c}$ ) into a charm pair. ${ }^{7}$ For this case the scaling variable becomes

$$
\begin{equation*}
\chi=x\left[1+\left(\frac{2 m_{c}}{Q}\right)^{2}\right] \tag{4}
\end{equation*}
$$

This rescaling is implemented in the $\mathrm{ACOT}_{\chi}$ scheme, for example [10-12]. The factor $\left(1+\left(2 m_{c}\right)^{2} / Q^{2}\right)$ represents a kinematic suppression factor which will suppress the charm process relative to the lighter quarks. Additionally, the $\chi$ scaling ensures the threshold kinematics $\left(W^{2}>4 m_{c}^{2}+M^{2}\right)$ are satisfied; while it is important to satisfy this condition for large $x$, this may prove too restrictive at small $x$ where the HERA data are especially precise. ${ }^{8}$

To encompass all the above results, we can define a general scaling variable $\chi(n)$ as

$$
\begin{equation*}
\chi(n)=x\left[1+\left(\frac{n m_{c}}{Q}\right)^{2}\right] \tag{5}
\end{equation*}
$$

where $n=\{0,1,2\}$. Here, $n=0$ corresponds to the massless result without rescaling, $n=1$ corresponds to the original Barnett slow rescaling, and $n=2$ corresponds to the $\chi$ rescaling.

## D. Phase space (kinematic) and dynamic mass

We now investigate the effects of separately varying the mass entering the $\chi(n)$ variable taking into account the phase space constraints and the mass value entering

[^183]the hard scattering cross section $\hat{\sigma}(m)$. We call the former mass parameter "phase space (kinematic) mass" and the latter "dynamic mass". 9

In Fig. 6(a) we display $F_{2}^{c}(x, Q)$ vs $Q$. The family of 3 curves shows the NLO ACOT calculation with $\chi(n)$ scaling using a zero dynamic mass for the hard scattering. We compare this with Fig. 6(b) which shows $F_{2}^{c}(x, Q)$ in the NLO ACOT scheme using a fixed $n=2$ scaling, but varying the mass used in the hard-scattering cross section. The upper (cyan) curves use a nonzero dynamic mass [ $\left.\hat{\sigma}\left(m_{c}=1.3\right)\right]$ and the lower (purple) curves have been obtained with a vanishing dynamic mass $\left[\hat{\sigma}\left(m_{c}=0\right)\right]$. We observe that the effect of the "dynamic mass" in $\hat{\sigma}\left(m_{c}\right)$ is only of consequence in the limited region $Q \gtrsim m$, and even in this region the effect is minimal. In contrast, the influence of the phase space (kinematic) mass shown in Fig. 6(a) is larger than the dynamic mass shown in Fig. 6(b). To highlight these differences, we scale the curves in Fig. 7 by the massless $n=2$ scaling result and plot bands that represent the variation of the dynamic and kinematic masses.

In conclusion, we have shown that (up to $\mathcal{O}\left(\alpha_{S}\right)$ ) the phase space mass dependence is generally the dominant contribution to the DIS structure functions. Assuming that this observation remains true at higher orders, it is possible to obtain a good approximation of the structure functions in the ACOT scheme at NNLO and $\mathrm{N}^{3} \mathrm{LO}$ using the massless Wilson coefficients together with a nonzero phase space mass entering via the $\chi(n)$ prescription.

## III. ACOT SCHEME BEYOND NLO

We have shown using the NLO full ACOT scheme that the dominant mass effects are those coming from the phase space which can be taken into account via a generalized slow-rescaling $\chi(n)$ prescription. Assuming that a similar relation remains true at higher orders, one can construct the following approximation to the ACOT result up to $\mathrm{N}^{3} \mathrm{LO}$ $\left(\mathcal{O}\left(\alpha_{S}^{3}\right)\right)$ :

$$
\begin{align*}
\operatorname{ACOT}\left[\mathcal{O}\left(\alpha_{S}^{0+1+2+3}\right)\right] \simeq & \operatorname{ACOT}\left[\mathcal{O}\left(\alpha_{S}^{0+1}\right)\right] \\
& +\mathrm{ZM}^{-\operatorname{VFNS}_{\chi(n)}}\left[\mathcal{O}\left(\alpha_{S}^{2+3}\right)\right] \tag{6}
\end{align*}
$$

In this equation, "ACOT" generically represents any variant of the ACOT scheme (ACOT, S-ACOT, S-ACOT ${ }_{\chi}$ ); for the results presented in Sec. IV, we will use the fully massive ACOT scheme with all masses retained out to NLO. The $\mathrm{ZM}^{2}-\mathrm{VFNS}_{\chi(n)}$ term uses the massless Wilson

[^184]
(a) Comparison of $F_{2}^{c}(x, Q)$ vs. $Q$ for the NLO ACOT calculation for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) using zero dynamic mass $[\hat{\sigma}(m=0)]$ to show the effect of $n$ scaling; from top to bottom $n=\{0,1,2\}$ (pink, black, purple).



(b) Comparison of $F_{2}^{c}(x, Q)$ vs. $Q$ for the NLO ACOT calculation for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). Here we keep the scaling fixed $n=2$ and compare the effect of varying the dynamic mass in the Wilson coefficient. The upper (cyan) curve uses a non-zero dynamic mass $[\widehat{\sigma}(m=1.3)]$ and the lower (purple) curve uses a zero dynamic mass $[\widehat{\sigma}(m=0)]$.

FIG. 6 (color online). Comparison of phase space (kinematic) \& dynamic mass effects.




FIG. 7 (color online). Comparison of kinematic \& dynamic mass effects for $F_{2}^{c}(x, Q)$ vs $Q$ for the NLO ACOT calculation for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). The curves are scaled by the massless $n=2$ result. The wider (yellow) band represents the variation of the kinematic mass of Fig. 6(a); note this band extends down to a ratio of 1.0. The narrower (blue) band is overlaid on the plot and represents the variation of the dynamic mass of Fig. 6(b).
coefficients at $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$ and $\mathcal{O}\left(\alpha \alpha_{S}^{3}\right)$ with the specified $\chi(n)$ scaling. ${ }^{10}$ Sample processes which contribute at this order are displayed in Fig. 8.

We use the $\mathrm{ZM}^{-V F N S}{ }_{\chi(n)}$ result in Eq. (6) to approximate the higher-order terms because not all the necessary massive Wilson coefficients at $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$ and $\mathcal{O}\left(\alpha \alpha_{S}^{3}\right)$ have been computed. There has been a calculation of neutral current electroproduction (equal quark masses, vector coupling) of heavy quarks at this order by Smith and van Neerven [13] in the FFNS which could be used to

[^185]obtain the massive Wilson coefficients in the S-ACOT scheme by applying appropriate collinear subtraction terms. However, for the original ACOT scheme it would then still be necessary to compute the massive Wilson coefficients for the heavy quark initiated subprocess at $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$. See Refs. [12,14] for details.

Using the result of Ref. [13], Thorne and Roberts developed an NLO variable-flavor-number scheme (VFNS) [7,15], and an improved NNLO formulation was presented in Ref. [16]. The fixed-order next-to-leading logs (FONLL) formalism was outlined in Ref. [17] and this was used to construct matched expressions for structure functions to NNLO [18]; implications of these results in the context of the NNPDF analysis were presented in Ref. [19]. An


FIG. 8. Sample Feynman diagrams contributing to DIS heavy quark production (from left): LO $\mathcal{O}\left(\alpha_{S}^{0}\right)$ quark-boson scattering $Q V \rightarrow Q, \mathrm{NLO} \mathcal{O}\left(\alpha_{S}^{1}\right)$ gluon-boson scattering $g V \rightarrow Q \bar{Q}$, NNLO $\mathcal{O}\left(\alpha_{S}^{2}\right)$ boson-gluon scattering $g V \rightarrow g Q \bar{Q}$, and $\mathrm{N}^{3} \mathrm{LO}$ $\mathcal{O}\left(\alpha_{S}^{3}\right)$ boson-gluon scattering $g V \rightarrow g g Q \bar{Q}$.
overview and comparison of these analyses was presented in the 2009 Les Houches report [20]. More recently, an NNLO S-ACOT- $\chi$ calculation was developed in Refs. [12,14]. For charge current case massive calculations are available at order $\mathcal{O}\left(\alpha \alpha_{S}\right)$ [21-23] and partial results at order $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$ [24]. Comparative analyses of these schemes are under investigation; however, this is beyond the scope of this paper.

Here, we argue that the massless Wilson coefficients at $\mathcal{O}\left(\alpha \alpha_{S}^{2}\right)$ together with a $\chi(n)$ prescription provide a very good approximation of the exact result. At worst, the maximum error would be of order $\mathcal{O}\left(\alpha \alpha_{S}^{2} \times\left[m^{2} / Q^{2}\right]\right)$. However, based on the arguments of Sec. II D we expect the inclusion of the phase space mass effects to contain the dominant higher order contributions so that the actual error should be substantially smaller.

The massless higher order coefficient functions for the DIS structure function $F_{2}$ via photon exchange can be found in Refs. [25-27] for $\mathcal{O}\left(\alpha_{S}^{1}\right)$, Refs. [28-30] for $\mathcal{O}\left(\alpha_{S}^{2}\right)$, and Ref. [31] for $\mathcal{O}\left(\alpha_{S}^{3}\right)$. For our numerical code we have used the $x$-space parameterization provided in Refs. [32,33] for $\mathcal{O}\left(\alpha_{S}^{2}\right)$, and Refs. [31,34] for $\mathcal{O}\left(\alpha_{S}^{3}\right)$.

The expressions for the structure function $F_{L}$ have been calculated in Refs. [29,35] for $\mathcal{O}\left(\alpha_{S}^{2}\right)$, and Ref. [31] for $\mathcal{O}\left(\alpha_{S}^{3}\right)$. In our FORTRAN code we have used the $x$-space parameterization provided in Refs. [32,36] for $\mathcal{O}\left(\alpha_{S}^{2}\right)$ and Ref. [36] for $\mathcal{O}\left(\alpha_{S}^{3}\right)$.

In order to calculate the inclusive structure functions $F_{2}$ and $F_{L}$ in the ZM-VFNS $\chi_{\chi}$ using these Wilson coefficients, plus- and delta-distributions have to be evaluated which is in principle straightforward. However, for the implementation of the slow-rescaling prescription it is necessary to decompose the Wilson coefficients into the contributions from different parton flavors. This step is nontrivial at $\mathcal{O}\left(\alpha_{S}^{2}\right)$ and beyond, and we therefore provide some details of our calculation in the Appendix B.

## A. Choice of $\boldsymbol{\chi}(\boldsymbol{n})$ rescaling

We now consider our choice for the appropriate generalized $\chi(n)$-rescaling variable.

In Table I we display the various rescalings of $\xi$ for the LO $\gamma Q \rightarrow Q$ process and the NLO $\gamma g \rightarrow Q \bar{Q}$ process. The "general" result is obtained by working out the detailed kinematics for the corresponding process [37].

The factor $\eta$ is the rescaling due to the hadronic mass $M$; notice that this factors out from the partonic mass dependence as it should [1]. For details see Appendix A.

The LO case with full massive kinematics has been computed in Ref. [37]. In the limit where the initial mass is small $\left(m_{1} \rightarrow 0\right)$, we recover the Barnett [9] slowrescaling result. Additionally, we obtain the curious result that for a neutral current equal mass case ( $m_{1}=m_{2}$ ) the rescaling is this same factor.

For the NLO gluon-induced process, the interpretation of the rescaling is straightforward; the phase space is simply suppressed by the total invariant mass of the final state $\left(m_{1}+m_{2}\right)$ compared to the scale $Q$. For the charged current case where we neglect $m_{1}$, we again obtain the standard rescaling factor. However, for the neutral current case $\left(m_{1}=m_{2}\right)$ we obtain a rescaling factor which is analogous to the $\chi$-scaling factor.

For the purposes of this study, we will vary the phase space mass using the $\chi(n)$ rescaling with $n=\{0,1,2\}$. While $n=0$ corresponds to the massless case (no rescaling), it is not obvious whether $n=1$ or $n=2$ is the preferred rescaling choice for higher orders. Thus, we

TABLE I. The massive rescaling factor for the LO quark-initiated process $\left(V q_{1} \rightarrow q_{2}\right)$, and the NLO gluon-initiated process ( $V g \rightarrow q_{1} \bar{q}_{2}$ ). The quarks $q_{1,2}$ have mass $m_{1,2}$, respectively, and $V$ represents the vector boson; $\gamma / Z$ for neutral current processes ( $m_{1}=m_{2}$ ), and $W^{ \pm}$for charged current processes $\left(m_{1} \neq m_{2}\right) . \eta$ is the scaling factor which depends on the hadronic mass $M$; see Appendix A for details. The triangle-function is defined as: $\Delta[a, b, c]=$

| $\sqrt{a^{2}+b^{2}+c^{2}-2(a b+b c+c a)}$. |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: |
| $\xi$ | General | $m_{1}=0$ | $m_{1}=m_{2}=m$ | $\chi$ scheme: |
| $w^{3}$ | $\eta\left[\frac{Q^{2}-m_{1}^{2}+m_{2}^{2}+\Delta\left[-Q^{2}, m_{1}^{2}, m_{2}^{2}\right]}{2 Q^{2}}\right]$ | $\eta\left[1+\frac{m_{2}^{2}}{Q^{2}}\right]$ | $\eta\left[1+\frac{m^{2}}{Q^{2}}\right]$ | $\eta\left[1+\frac{(2 m)^{2}}{Q^{2}}\right]$ |
|  | $\eta\left[1+\left(\frac{m_{1}+m_{2}}{Q}\right)^{2}\right]$ | $\eta\left[1+\frac{m_{2}^{2}}{Q^{2}}\right]$ | $\eta\left[1+\frac{(2 m)^{2}}{Q^{2}}\right]$ | $\eta\left[1+\frac{(2 m)^{2}}{Q^{2}}\right]$ |



FIG. 9 (color online). $\quad F_{2, L}$ vs $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). The three lines show the scaling variable: $n=\{0,1,2\}$ (red, green, blue). We observe the effect of the $n$ scaling is negligible except for very small $Q$ values.
will use the range between $n=1$ and $n=2$ as a measure of our theoretical uncertainty arising from this ambiguity.

## IV. RESULTS

We now present the results of our calculation extending the ACOT scheme to NNLO and $\mathrm{N}^{3} \mathrm{LO}$. As outlined in Eq. (6), we will use the fully massive ACOT scheme for the LO and NLO contributions, and combine this with the ZM-VFNS supplemented with the $\chi$-rescaling prescription to approximate the higher order terms. We will use the QCDNUM program [38] with the VFNS evolved with the DGLAP kernels at NNLO to generate our PDFs from an initial distribution based on the Les Houches benchmark set [39]; this ensures that our heavy quark PDFs are consistently evolved so that the heavy quark initiated LO terms properly match the corresponding SUB contribution. At NNLO the proper matching conditions across flavor thresholds introduces discontinuities in the PDFs which are incorporated in the QCDNUM program; we discuss this in detail in Appendix C. We choose $m_{c}=1.3 \mathrm{GeV}, m_{b}=$ $4.5 \mathrm{GeV}, \alpha_{S}\left(M_{Z}\right)=0.118$. We note that the QCDNUM ZM-STFN package has the massless Wilson coefficients computed up to $\mathrm{N}^{3} \mathrm{LO}$; we cross checked our implementation of ACOT in the massless limit with QCDNUM, and they agree precisely.

## A. Effect of $\boldsymbol{\chi}(\boldsymbol{n})$ scaling

In Figs. 9(a) and 9(b) we display the structure functions $F_{2}$ and $F_{L}$, respectively, for selected $x$ values as a function of $Q$. Each plot has three curves which are computed using
$n$ scalings of $\{0,1,2\}$. We observe that the effect of the $n$ scaling is negligible except for very small $Q$ values. This result is in part because the heavy quarks are only a fraction of the total structure function, and the effects of the $n$ scaling are reduced at larger $Q$ values.

In Fig. 10 we magnify the small $Q$ region of $F_{L}$ of Fig. 9 for $x=10^{-5}$, where the effects of using different scalings are largest. We can see that for inclusive observables, the $n=1$ and $n=2$ scalings give nearly identical results, but they differ from the massless case ( $n=0$ ). This result, together with the observation that at NLO kinematic mass effects are dominant, suggests that the error we have in our approach is relatively small and approximated by the band between $n=1$ and $n=2$ results.


FIG. 10 (color online). Enlargement of Fig. 9(b) for $x=10^{-5}$ showing the small $Q$ region. Here we can distinguish plots for different scalings; from top to bottom we have $n=\{0,1,2\}$ (red, green, blue).


FIG. 11 (color online). Effect of $\chi(n)$ scaling for $n=\{0,1,2\}$ (left to right) at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-3}\right\}$. Reading from the bottom we have fractional contribution for each quark flavor to $F_{2, L}^{j} / F_{2, L}$ vs $Q$ from $\{u, d, s, c, b\}$ (green, blue, cyan, magenta, pink).

## B. Flavor decomposition of $\boldsymbol{\chi}(\boldsymbol{n})$ scaling

We can investigate the effects of the $\chi(n)$ scaling in more details by examining the flavor decomposition of the structure functions.

In Figs. 11(a) and 11(b) we display the fractional contributions of quark flavors to the structure functions $F_{2, L}$ for selected $n$-scaling values as a function of $Q$. Flavor decomposition of inclusive structure functions is defined in Appendix B in Eqs. (B1) and (B2). We observe the $n$ scaling reduces the relative contributions of charm and bottom at low $Q$ scales. For example, without any $n$ scaling ( $n=0$ ) we find the charm and bottom quarks contribute an unusually large fraction at very low scales $\left(Q \sim m_{c}\right)$ as they are (incorrectly) treated as massless partons in this region. The result of the different $n$ scalings $(n=1,2)$ is to introduce a kinematic penalty which properly suppresses the contribution of these heavy quarks in the low $Q$ region. In the following, we will generally use the $n=2$ scaling for our comparisons.

## C. $\boldsymbol{F}_{\mathbf{2}, L}$ initial-state flavor decomposition

In Figs. 12(a) and 12(b) we display the fractional contributions for the initial-state quarks $(i)$ to the structure functions $F_{2}$ and $F_{L}$, ${ }^{11}$, respectively, for selected $x$ values as a function of $Q$; here we have used $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{g, u, d, s, c, b\}$. Although this decompo-

[^186]sition is not physically observable, it is instructive to see which PDFs are dominantly influencing the result. We observe that for large $x$ and low $Q$ the heavy flavor contributions are minimal. For example, for $x=10^{-1}$ we see the contribution of the $u$-quark comprises $\sim 80 \%$ of the $F_{2}$ structure function at low $Q$. In contrast, at $x=10^{-5}$ and large $Q$ we see the $F_{2}$ contributions of the $u$-quark and $c$-quark are comparable (as they both couple with a factor $4 / 9$ ), and the $d$-quark and $s$-quark are comparable (as they both couple with a factor $1 / 9$ ).

It is notable that the gluon contribution to $F_{L}$ is significant. For $x=10^{-1}$ this is roughly $40 \%$ throughout the $Q$ range, and can be even larger for smaller $x$ values.

## D. $\boldsymbol{F}_{\mathbf{2}, L}$ final-state flavor decomposition

In Figs. 13(a) and 13(b) we display the fractional contributions for the final-state quarks $(j)$ to the structure functions $F_{2}$ and $F_{L}$, respectively, for selected $x$ values as a function of $Q$; here we have used $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{u, d, s, c, b\}$. Again, we observe that for large $x$ and low $Q$ the heavy flavor contributions are minimal, but these can grow quickly as we move to smaller $x$ and larger $Q$.

## E. Comparison of LO, NLO, NNLO, $\mathrm{N}^{\mathbf{3}} \mathrm{LO}$

In Fig. 14(a) we display the results for $F_{2}$ vs $Q$ computed at various orders. For large $x$ (cf. $x=0.1$ ) we find the perturbative calculation is particularly stable; we see that the LO result is within $20 \%$ of the others at small $Q$, and


FIG. 12 (color online). Fractional flavor decomposition of "initial-state" $F_{2, L}^{i} / F_{2, L}$ vs $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for $n=2$ scaling. Reading from the bottom, we plot the cumulative contributions to $F_{2, L}$ from $\{g, u, d, s, c, b\}$, (red, green, blue, cyan, magenta, pink).


FIG. 13 (color online). Fractional contribution for each quark flavor to $F_{2, L}^{j} / F_{2, L}$ vs $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right). Results are displayed for $n=2$ scaling. Reading from the bottom, we have the cumulative contributions from the $\{u, d, s, c, b\}$ (green, blue, cyan, magenta, pink).
within $5 \%$ at large $Q$. The NLO is within $2 \%$ at small $Q$, and indistinguishable from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ for $Q$ values above $\sim 10 \mathrm{GeV}$. The NNLO and $\mathrm{N}^{3} \mathrm{LO}$ results are essentially identical throughout the kinematic range. For
smaller $x$ values $\left(10^{-3}, 10^{-5}\right)$ the contribution of the higher order terms increases. Here, the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ coincide for $Q$ values above $\sim 5 \mathrm{GeV}$, but the NLO result can differ by $\sim 5 \%$.


FIG. 14 (color online). $\quad F_{2, L}$ vs $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for $n=2$ scaling.

In Fig. 14(b) we display the results for $F_{L}$ vs $Q$ computed at various orders. In contrast to $F_{2}$, we find the NLO corrections are large for $F_{L}$; this is because the LO $F_{L}$ contribution (which violates the Callan-Gross relation) is suppressed by $\left(m^{2} / Q^{2}\right)$ compared to the dominant gluon contributions which enter at NLO. Consequently, we observe (as expected) that the LO result for $F_{L}$ receives large contributions from the higher order terms. ${ }^{12}$ Essentially, the NLO is the first nontrivial order for $F_{L}$, and the subsequent contributions then converge. For example, at large $x$ (cf. $x=0.1$ ) for $Q \sim 10 \mathrm{GeV}$ we find the NLO result yields $\sim 60$ to $80 \%$ of the total, the NNLO is a $\sim 20 \%$ correction, and the $\mathrm{N}^{3} \mathrm{LO}$ is a $\sim 10 \%$ correction. For lower $x$ values $\left(10^{-3}, 10^{-5}\right)$ the convergence of the perturbative series improves, and the NLO results is within $\sim 10 \%$ of the $\mathrm{N}^{3} \mathrm{LO}$ result. Curiously, for $x=10^{-5}$ the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ roughly compensate each other so that the NLO and the $\mathrm{N}^{3} \mathrm{LO}$ match quite closely for $Q \geq 2 \mathrm{GeV}$.

While the calculation of $F_{L}$ is certainly more challenging, examining Fig. 1 we see that for most of the relevant kinematic range probed by HERA the theoretical calculation is quite stable. For example, in the high $Q^{2}$ region where HERA is probing intermediate $x$ values $\left(x \sim 10^{-3}\right)$ the spread of the $\chi(n)$ scalings is small. The challenge

[^187]arises in the low $Q$ region $(Q \sim 2 \mathrm{GeV})$ where the $x$ values are $\sim 10^{-4}$; in this region, there is some spread between the various curves at the lowest $x$ value $\left(\sim 10^{-5}\right)$, but for $x \sim 10^{-3}$ this is greatly reduced.

## V. CONCLUSIONS

We extended the ACOT calculation for DIS structure functions to $\mathrm{N}^{3} \mathrm{LO}$ by combining the exact ACOT scheme at NLO with a $\chi(n)$ rescaling; this allows us to include the leading mass dependence at NNLO and $\mathrm{N}^{3} \mathrm{LO}$. Using the full ACOT calculation at NLO, we demonstrated that the heavy quarks mass dependence for the DIS structure functions is dominated by the kinematic mass contributions, and this can be implemented via a generalized $\chi(n)$-rescaling prescription.

We studied the $F_{2}$ and $F_{L}$ structure functions as a function of $x$ and $Q$. We examined the flavor decomposition of these structure functions, and verified that the heavy quarks were appropriately suppressed in the low $Q$ region. We found the results for $F_{2}$ were very stable across the full kinematic range for $\{x, Q\}$, and the contributions from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ terms were small. For $F_{L}$, the higher order terms gave a proportionally larger contribution (due to the suppression of the LO term from the Callan-Gross relation); nevertheless, the contributions from the NNLO and $\mathrm{N}^{3}$ LO terms were generally small in the region probed by HERA.

The result of this calculation was to obtain precise predictions for the inclusive $F_{2}$ and $F_{L}$ structure functions which can be used to analyze the HERA data.

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## APPENDIX A: KINEMATIC RELATIONS

## 1. Target mass contributions

In the DIS process, the effect of the target mass $(M)$ on the scaling variable is a multiplicative correction factor

$$
\begin{equation*}
\eta=\frac{2 x}{1+\sqrt{1+\frac{4 x^{2} M^{2}}{Q^{2}}}} \rightarrow \underset{M \rightarrow 0}{\rightarrow} x\left[1-\left(\frac{x M}{Q}\right)^{2}\right]+\ldots \tag{Al}
\end{equation*}
$$

This is used in Table I to modify the scaling variable [1,37].

## 2. Barnett scaling

If we consider the charged-current DIS process for charm production, this takes place via the subprocess $W^{+}(q) s(\xi P) \rightarrow c(k)$. If we impose 4-momentum conservation, we have $(q+\xi P)^{2}=k^{2}=m_{c}^{2}$. Defining $q^{2}=$ $-Q^{2}$ and $x=Q^{2} /(2 p \cdot q)$, we obtain the traditional "slow rescaling" relation [9]

$$
\xi=x\left(1+\frac{m_{c}^{2}}{Q^{2}}\right)
$$

which was used in Eq. (3).

## 3. $\hat{W}$ constraints

If we compute the invariant mass $\hat{W}$ of a boson of momentum $q$ scattering from a light parton $a$ of momentum $p_{a}=\xi P$, we find [14]

$$
\begin{equation*}
\hat{W}=\left(p_{a}+q\right)^{2}=Q^{2}(\xi / x-1) . \tag{A2}
\end{equation*}
$$

If the partonic final state has a minimum invariant mass $\hat{W}_{\text {min }}=4 m^{2}$, then $\xi$ is constrained by

$$
\begin{equation*}
1 \geq \xi \geq \chi \geq x \tag{AB}
\end{equation*}
$$

where $\chi=x\left(1+4 m^{2} / Q^{2}\right)$. This is the relation used in Eq. (4). This choice will ensure $\hat{W} \geq \hat{W}_{\text {min }}$ is satisfied. While this constraint is important in the large $x$ region,
this may be too restrictive in the small $x$ region-especially as this is the region where the HERA data is very precise.

## APPENDIX B: DECOMPOSITION OF THE WILSON COEFFICIENTS

In this appendix we present the decomposition of the Wilson coefficients used to implement the scheme. We will need to decompose the structure function $F$ in terms of the individual partonic contributions,

$$
\begin{equation*}
F=\sum_{i=0}^{5} \sum_{j=1}^{6} F^{i j} \tag{Bi}
\end{equation*}
$$

where the indices $i$ and $j$ represent initial and final-state partons, respectively, (see captions of Figs. 15-24). More specifically, $i=0$ denotes a gluon and $i, j=1,2,3, \ldots$ denotes $u, d, s, \ldots$ quarks and antiquarks. A top quark PDF ( $i=6$ ) is not included in this study.

Let us consider the heavy quark structure functions $F_{2, L}^{c}$ as an example. This is obtained by requiring that there is a charm in the initial state while summing over the final-state flavors up to and including charm in Eq. (B1), or by


FIG. 15. $\mathcal{O}\left(\alpha_{S}^{0}\right)-\gamma^{*} q_{i} \rightarrow q_{i}$. Contributes to $C_{a, q}^{\mathrm{ns}}$ (and hence to $C_{a, q}^{\mathrm{s}}$ ) but not to $C_{a, q}^{\mathrm{ps}}$.


FIG. 16. $\mathcal{O}\left(\alpha_{S}^{1}\right)-\gamma^{*} q_{i} \rightarrow q_{i} g$. Contributes to $C_{a, q}^{\mathrm{ns}}$ (and hence to $C_{a, q}^{\mathrm{s}}$ ) but not to $C_{a, q}^{\mathrm{ps}}$. This contribution does not depend on $n_{f}$.


FIG. 17. $\mathcal{O}\left(\alpha_{S}^{1}\right)-\gamma^{*} g \rightarrow q_{j} \bar{q}_{j}$.


FIG. 18. $\mathcal{O}\left(\alpha_{S}^{2}\right)-\gamma^{*} q_{i} \rightarrow q_{i} g g$. Contributes to $C_{a, q}^{\mathrm{ns}}$ (and hence to $C_{a, q}^{\mathrm{s}}$ ) but not to $C_{a, q}^{\mathrm{ps}}$. This part is independent of $n_{f}$.


FIG. 19. $\mathcal{O}\left(\alpha_{S}^{2}\right) — \gamma^{*} g \rightarrow q_{j} \bar{q}_{j} g$.
requiring that there is a charm in the final-state and summing over the initial flavors up to and including charm. Thus, we obtain:

$$
\begin{equation*}
F^{c}=\sum_{i=0}^{3} F^{i 4}+\sum_{j=1}^{3} F^{4 j}+F^{44} \tag{B2}
\end{equation*}
$$

The case where the initial and final-state are both charm quarks $\left(F^{44}\right)$ has been written explicitly in the equation to avoid double counting this contribution. ${ }^{13}$ The first sum in Eq. (B2) includes cases, as in Fig. 20, where the incoming quark is a light quark while the charm quark is one of the quarks in the quark antiquark pair.

In order to obtain the required decomposition, there are some manipulations that need to be performed to transform

[^188]
(a) Contribution proportional to $n_{f}$ for $C_{a, q}^{\mathrm{ps}}$.

(b) Contribution proportional to $n_{f}$ for $C_{a, q}^{\mathrm{ns}}$.

FIG. 20. $\mathcal{O}\left(\alpha_{S}^{2}\right)-\gamma^{*} q_{i} \rightarrow q_{i} q_{j} \bar{q}_{j}$.


FIG. 21. $\mathcal{O}\left(\alpha_{S}^{3}\right)-\gamma^{*} q_{i} \rightarrow q_{i} g g g$. Contribution to $C_{a, q}^{\mathrm{ns}}$ not proportional to $n_{f}$.
from the singlet ( $s$ ), nonsinglet ( $n s$ ), and purely singlet $(p s)$ structure function combinations found in the literature into individual partonic components.

The general expression for the structure function is given by:

$$
\begin{equation*}
x^{-1} F_{a}=q_{n s} \otimes C_{a, q}^{\mathrm{ns}}+\left\langle e^{2}\right\rangle\left(q_{\mathrm{s}} \otimes C_{a, q}^{\mathrm{s}}+g \otimes C_{a, g}\right) \tag{B3}
\end{equation*}
$$

where $a=\{2, L\}$, and
$q_{\mathrm{ns}}=\sum_{i=1}^{n_{f}}\left(e_{i}^{2}-\left\langle e^{2}\right\rangle\right) q_{i}^{+}, \quad q_{\mathrm{s}}=\sum_{i=1}^{n_{f}} q_{i}^{+}$,
$q_{i}^{+}=q_{i}+\bar{q}_{i}, \quad\left\langle e^{2}\right\rangle=\left\langle e^{2}\right\rangle^{\left(n_{f}\right)}=\frac{1}{n_{f}} \sum_{i=1}^{n_{f}} e_{i}^{2}$,


FIG. 22. $\mathcal{O}\left(\alpha_{S}^{3}\right)-\gamma^{*} g \rightarrow q_{j} \bar{q}_{j} g g$.
and $C_{a, q}^{\mathrm{ns}}, C_{a, q}^{\mathrm{s}}, C_{a, g}$ are the Wilson coefficients. From Eq. (B4) one can extract the contribution from a single initial-state quark as

$$
\begin{equation*}
x^{-1} F_{a, q_{i}}=q_{i}^{+} \otimes\left[e_{i}^{2} C_{a, q}^{\mathrm{ns}}+\left\langle e^{2}\right\rangle C_{a, q}^{\mathrm{ps}}\right] \tag{B5}
\end{equation*}
$$

where $C_{a, q}^{\mathrm{ps}}$ is

$$
\begin{equation*}
C_{a, q}^{\mathrm{ps}}=C_{a, q}^{\mathrm{s}}-C_{a, q}^{\mathrm{ns}} . \tag{B6}
\end{equation*}
$$

To further decompose Eq. (B5) into the different finalstate contributions, we examine the diagrams that contribute to the nonsinglet and purely singlet coefficients. Diagrams in which the photon couples to the incoming quark contribute to $C_{a, q}^{\mathrm{ns}}$ (Figs. 15, 16, 18, and 20(b), etc.), whereas the diagrams where the photon does not couple to

(a) Contribution proportional to $n_{f}$ for $C_{a, q}^{\mathrm{ps}}$.

(b) Contribution proportional to $n_{f}$ for $C_{a, q}^{\mathrm{ns}}$.

FIG. 23. $\mathcal{O}\left(\alpha_{S}^{3}\right)-\gamma^{*} q_{i} \rightarrow q_{i} q_{j} \bar{q}_{j} g$.


FIG. 24. $\mathcal{O}\left(\alpha_{S}^{3}\right)-\gamma^{*} g \rightarrow q_{j} \bar{q}_{j} q_{k} \bar{q}_{k}$.
the incoming quark contribute to $C_{a, q}^{\mathrm{ps}}$; these contributions appear for the first time at $\mathcal{O}\left(\alpha_{S}^{2}\right)$ in Figs. 20(a) and 23(a). Separating out the final-state quark from Eq. (B5) we obtain:

$$
\begin{align*}
x^{-1} F_{a}^{i j}= & q_{i}^{+} \otimes\left\{e _ { i } ^ { 2 } \left[C_{a, q}^{\mathrm{ns}}\left(n_{f}=0\right) \delta_{i j}\right.\right. \\
& \left.+C_{a, q}^{\mathrm{ns}}(j)-C_{a, q}^{\mathrm{ns}}(j-1)\right] \\
& \left.+\left\langle e^{2}\right\rangle^{(j)} C_{a, q}^{\mathrm{ps}}(j)-\left\langle e^{2}\right\rangle^{(j-1)} C_{a, q}^{\mathrm{ps}}(j-1)\right\} . \tag{B7}
\end{align*}
$$

We have introduced $\delta_{i j}$ in the nonsinglet contribution to account for contributions in which the photon couples to the initial and final-state quark. When this is not the case, [i.e., in all purely singlet contributions and in nonsinglet contributions such as the ones in Fig. 20(a)], the difference of the coefficient functions with $n_{f}=j$ and $n_{f}=j-1$ flavors is taken.

Some comments are in order:
(i) We have verified analytically and numerically that one recovers Eq. (B5) when summing over the final state quark partons $\left(j=1, \ldots, n_{f}\right)$ in Eq. (B7).
(ii) The corresponding decomposition for the gluoninitiated subprocesses is simpler than the one in Eq. (B7) since there are only purely singlet contributions:

$$
\begin{equation*}
x^{-1} F_{a}^{0 j}=g \otimes\left\{\left\langle e^{2}\right\rangle^{(j)} C_{a, g}(j)-\left\langle e^{2}\right\rangle^{(j-1)} C_{a, g}(j-1)\right\} . \tag{B8}
\end{equation*}
$$

(iii) We remark that the decomposition in Eq. (B7) also includes the contributions from virtual diagrams to the Wilson coefficients. As has been discussed in the literature [40], such a decomposition is ambiguous at $\mathcal{O}\left(\alpha_{S}^{2}\right)$ and beyond due to the treatment of heavy quark loops contributing to the light quark structure functions. However, numerically the ambiguous terms are small and it is standard to analyze the heavy quark structure functions $F_{2, L}^{c}$
and $F_{2, L}^{b}$ in addition to the inclusive structure functions $F_{2, L}$ without any further prescription.
For the general neutral current case (including Z-boson exchange), the electromagnetic couplings should be replaced by electroweak couplings as follows:

$$
\begin{equation*}
e_{i}^{2} \rightarrow a_{q_{i}}^{+}=e_{i}^{2}-2 e_{i} v_{e} v_{q} \chi_{Z}+\left(v_{e}^{2}+a_{e}^{2}\right)\left(v_{q}^{2}+a_{q}^{2}\right) \chi_{Z}^{2} \tag{B9}
\end{equation*}
$$

where

$$
\begin{equation*}
v_{f}=T_{f}^{3}-2 Q_{f} \sin ^{2} \theta_{W}, \quad a_{f}=T_{3}^{f} \tag{B10}
\end{equation*}
$$

are the standard (axial-)vector couplings of the $Z$-boson to the leptons $(f=e)$ and quarks $(f=q)$. Furthermore, $\chi_{Z}$ is the ratio of the $Z$-boson propagator with respect to the photon propagator including additional coupling factors:

$$
\begin{equation*}
\chi_{Z}=\frac{G_{F} M_{Z}^{2}}{2 \sqrt{2} \pi \alpha_{e m}} \frac{Q^{2}}{Q^{2}+M_{Z}^{2}} . \tag{B11}
\end{equation*}
$$

Finally, the average squared charge is modified as

$$
\begin{equation*}
\left\langle e^{2}\right\rangle^{\left(n_{f}\right)} \rightarrow a^{+}\left(n_{f}\right)=\frac{1}{n_{f}} \sum_{i=1}^{n_{f}} a_{q_{i}}^{+} . \tag{B12}
\end{equation*}
$$

## APPENDIX C: MATCHING ACROSS HEAVY FLAVOR THRESHOLDS

As we compute at higher orders, we find the matching conditions of the PDFs become discontinuous at $\mathcal{O}\left(\alpha_{s}^{2}\right)$ (NNLO), and the matching of the $\overline{\mathrm{MS}} \alpha_{s}(\mu)$ becomes discontinuous at $\mathcal{O}\left(\alpha_{s}^{3}\right)\left(\mathrm{N}^{3} \mathrm{LO}\right)$.

While the discontinuities in the PDFs and $\alpha_{s}$ (which are unphysical quantities) persist at all orders, physical observables (such as cross sections and structure functions) will match across thresholds up to the computed order of the perturbation theory; for example, a physical observable in an $N$-flavor and an $(N+1)$-flavor scheme will match up to higher order terms when computed to order $\alpha_{s}^{M}$ in the perturbation expansion:

$$
\sigma^{N}=\sigma^{N+1}+\mathcal{O}\left(\alpha_{s}^{M+1}\right)
$$

As it is not immediately obvious how the discontinuities cancel order by order, we shall examine a NNLO numeric case, and also a simple analytic example.

## 1. Discontinuities across the flavor transition

To illustrate the behavior of the discontinuities, we will work at NNLO where the DGLAP evolution and the flavorthreshold boundary conditions have been computed and implemented. ${ }^{14}$ Since $\mu=m_{c}$ is often used for the initial

[^189]evolution scale, we will focus on the transition from $N_{F}=4$ to $N_{F}=5$ flavors at $\mu=m_{b}$.

The matching conditions across flavor thresholds can be summarized as [41]

$$
\begin{equation*}
f_{a}^{N+1}=A_{a b} \otimes f_{b}^{N} \tag{C1}
\end{equation*}
$$

where $f^{N}$ and $f^{N+1}$ are the PDFs for $N$ and $N+1$ flavors, and $A_{a b}$ can be expanded perturbatively. In the VFNS for $\mu<m_{b}$, the $b$-quark PDF is zero and the gluon PDF is finite and positive. Using Eq. (C1) for $\mu>m_{b}$, we find the $b$-quark is negative for $\mu \sim m_{b}$, and it becomes more negative as we move to smaller $x$. In contrast, the gluon has a positive discontinuity as it must to ensure the momentum sum rule is satisfied.

## 2. The $\boldsymbol{b}$-quark flavor transition

Although these discontinuities are too small to be noticeable in the figures of Sec. IV, in Fig. 25 we have magnified the axes so the discontinuities are visible. Here, we display $F_{2}$ and $F_{L}$ for a selection of $x$ values.

The first general feature we notice in Fig. 25 is that the size of the discontinuity generally grows as we go to smaller $x$ values. This is consistent with the fact that the discontinuity computed by Eq. (C1) also grows for smaller $x$. We display the results for a selection of $n$-scaling values; note that the uncertainty arising from the discontinuity is typically on the order of the difference due to the choice of scaling.

Another feature that is most evident for the series of $F_{L}$ plots (Fig. 25(b)) is that the discontinuity can change sign for different $x$ values. This can happen because the mix of quark and gluon initiated terms is changing as a function of $x$.

This observation is key to understanding how the (unphysical) PDFs may have a relatively large discontinuity, while the effect on the physical quantities (such as $\sigma$ and $F_{2, L}$ ) is moderated. Because physical quantities will contain a sum of gluon and quark initiated contributions, and because the discontinuity of the quark and gluon PDFs have opposite signs, the discontinuities of the quark and gluon PDFs can partially cancel so that the physical quantity may have a reduced discontinuity.

This discontinuity, in part, reflects the theoretical uncertainty of the perturbation theory at a given order. As we compute the physical observables to higher and higher orders, this discontinuity will be reduced even though the discontinuity in the PDFs and $\alpha_{s}$ remain. We will demonstrate this mechanism in the following.

## C. A "Toy" example at NLO

We now illustrate how the cancellation of the quark and gluon PDF discontinuities work analytically using a toy calculation.


(a) $F_{2}$ vs. $Q$ for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for different $n$ scalings.

(b) $F_{L}$ vs. $Q$ for $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for different $n$ scalings.

FIG. 25 (color online). Discontinuity for $F_{2}, F_{L}$ at NNLO in the region of the bottom mass, $m_{b}=4.5 \mathrm{GeV}$.

Expanding Eq. (C1) in the region of $\mu=m_{b}$ we have:

$$
\begin{align*}
& f_{b}^{5}=\left\{0+\frac{\alpha_{s}}{2 \pi} P_{q g}\left(L+a_{q g}\right)+O\left(\alpha_{s}^{2}\right)\right\} \otimes f_{g}^{4}  \tag{C2}\\
& f_{g}^{5}=\left\{1+\frac{\alpha_{s}}{2 \pi} P_{g g}\left(L+a_{g g}\right)+O\left(\alpha_{s}^{2}\right)\right\} \otimes f_{g}^{4}
\end{align*}
$$

where $L=\ln \left(\mu^{2} / m_{b}^{2}\right)$. It happens that the constant terms $a_{i j}$ in Eq. ( C 2$)$ are zero at $\mathcal{O}\left(\alpha_{s}^{1}\right)$ in the $\overline{\mathrm{MS}}$ scheme; this is not due to any underlying symmetry, and in fact at $\mathcal{O}\left(\alpha_{s}^{2}\right)$ these terms are nonzero. Because $a_{i j}$ are zero, if we perform the matching at $\mu=m_{b}$, we find that the gluon PDF is continuous $f_{b}^{5}\left(x, m_{b}\right)=f_{g}^{4}\left(x, m_{b}\right)$, and the bottom PDF starts from zero $f_{b}^{5}\left(x, m_{b}\right)=0$.

$$
\text { a. If } a_{i j} \text { was nonzero at } \mathcal{O}\left(\alpha_{s}^{1}\right)
$$

To illustrate how the discontinuities cancel in the ACOT renormalization scheme, we will suppose (for this toy calculation) that the constant terms $\left(a_{i j}\right)$ in the matching conditions are nonvanishing at order $\alpha_{s}^{1}$; thus, the gluon and bottom PDFs will now have $\mathcal{O}\left(\alpha_{s}^{1}\right)$ discontinuities, but the physical observables computed with different $N_{F}$ values will still match up to $\mathcal{O}\left(\alpha_{s}^{2}\right)$.

In the ACOT scheme, the total cross section can be decomposed as: $\sigma_{\mathrm{TOT}}=\sigma_{\mathrm{LO}}+\sigma_{\mathrm{NLO}}-\sigma_{\mathrm{SUB}}$, where $\sigma_{\mathrm{LO}}$ represents $\gamma b \rightarrow b, \sigma_{\mathrm{NLO}}$ represents $\gamma g \rightarrow b \bar{b}$, and $\sigma_{\text {SUB }}$ represents the $(g \rightarrow b) \otimes(\gamma b \rightarrow b)$ "subtraction" contribution. ${ }^{15}$ We will now perturbatively compute $\sigma_{\text {TOT }}$ in the region $\mu \sim m_{b}$ for both $N_{F}=4$ and $N_{F}=5$.

[^190]
## b. ACOT for $N_{F}=4$

For $\mu<m_{b}$, we have $N_{F}=4$ and $f_{b}=0$; thus, $\sigma_{\mathrm{LO}}$ and $\sigma_{S U B}$ vanish, and we have:

$$
\sigma_{\mathrm{TOT}}^{N_{F}=4}=\sigma_{\mathrm{NLO}}=C^{1} \otimes f_{g}^{4}+O\left(\alpha_{s}^{2}\right)
$$

where $C^{1}$ represents the $\mathcal{O}\left(\alpha_{s}^{1}\right)$ process $\gamma g \rightarrow b \bar{b}$.

$$
\text { c. ACOT for } N_{F}=5
$$

For $\mu>m_{b}$, we have $N_{F}=5$ and $f_{b} \neq 0$. For the contributions we have:

$$
\begin{aligned}
\sigma_{\mathrm{LO}}= & C^{0} \otimes f_{b}^{5} \simeq C^{0} \otimes\left\{0+\frac{\alpha_{s}}{2 \pi} P_{q g}\left(L+a_{q g}\right)\right\} \otimes f_{g}^{4} \\
\sigma_{\mathrm{NLO}}= & C^{1} \otimes f_{g}^{5} \simeq C^{1} \otimes\left\{1+\frac{\alpha_{s}}{2 \pi} P_{g g}\left(L+a_{g g}\right)\right\} \otimes f_{g}^{4} \\
\sigma_{\mathrm{SUB}}= & C^{0} \otimes \tilde{f}_{g \rightarrow q} \otimes f_{g}^{5} \simeq C^{0} \otimes\left\{\frac{\alpha_{s}}{2 \pi} P_{q g}\left(L+a_{q g}\right)\right\} \\
& \otimes\left\{1+\frac{\alpha_{s}}{2 \pi} P_{g g}\left(L+a_{g g}\right)\right\} \otimes f_{g}^{4}
\end{aligned}
$$

Keeping terms to $\mathcal{O}\left(\alpha_{s}^{1}\right)$ we have:

$$
\sigma_{\mathrm{TOT}}^{N_{F}=5}=\sigma_{\mathrm{LO}}+\sigma_{\mathrm{NLO}}-\sigma_{\mathrm{SUB}}=C^{1} \otimes f_{g}^{4}+O\left(\alpha_{s}^{2}\right)
$$

Notice that the discontinuity introduced by $a_{q g}$ in the PDFs is canceled by $a_{q g}$ from the SUB contribution. ${ }^{16}$

[^191]
## d. Comparison of $N_{F}=5$ and $N_{F}=4$

Comparing the $N_{F}=5$ and $N_{F}=4$ results, we find

$$
\sigma_{\mathrm{TOT}}^{N_{F}=5}=\sigma_{\mathrm{TOT}}^{N_{F}=4}+O\left(\alpha_{s}^{2}\right)
$$

so that the total physical results match up the order of the perturbation theory.

In the above illustration, we have retained the log terms $(L)$; the cancellation of the logs is ensured in a well defined renormalization scheme, and the $a_{i j}$ constant terms get carried along with the logs and will thus cancel order by order.

Therefore, the discontinuity of the physical quantities ( $\sigma, F_{2, L}$ ) reflects the perturbative uncertainty, and this will be systematically reduced at higher orders.
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# THE SM AND NLO MULTILEG AND SM MC WORKING GROUPS: Summary Report 

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#### Abstract

The 2011 Les Houches workshop was the first to confront LHC data. In the two years since the previous workshop there have been significant advances in both soft and hard QCD, particularly in the areas of multi-leg NLO calculations, the inclusion of those NLO calculations into parton shower Monte Carlos, and the tuning of the non-perturbative parameters of those Monte Carlos. These proceedings describe the theoretical advances that have taken place, the impact of the early LHC data, and the areas for future development.


Report of the SM and NLO Multileg and SM MC Working Groups for the Workshop "Physics at TeV Colliders", Les Houches, France, 31 May-8 June, 2011.

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## Part I

## INTRODUCTION

The workshop in 2011 was the first for which the long-awaited LHC data (at 7 TeV ) was available for analysis and comparison to theory. Even though of limited statistical power compared to the ultimate goals of the LHC, this data accesses a very wide kinematic range, and probes regions where multiple scales are important. The presence of large scales for some processes, on the TeV level, points to the importance of electroweak corrections, which have been calculated only for some of the important processes. The first hints of a Higgs boson have now been observed. In order to search for signs of New Physics, as well as to completely understand the Standard Model at the LHC, it is important to understand the perturbative framework at the LHC. The data taken so far provides many challenges for perturbative QCD predictions; and it is clear that New Physics, if it is present in current data, is hiding well.

On the theoretical side, there has been a great deal of productivity in the area of multi-particle calculations at next-to-leading order (NLO) and next-to-next-to-leading order (NNLO). NLO is the first order at which the normalization, and in some cases the shape, of perturbative cross sections can be considered reliable [1]. A full understanding for both Standard Model and beyond the Standard Model physics at the LHC requires the development of fast, reliable programs for the calculation of multi-parton final states at NLO. There have been many advances in the development of NLO techniques, especially in the area of automation $[2,3,4,5,6,7,8,9,10,11,12]$.

Some of these approaches also allow for relatively easy [13, 14, 12] and/or automatic [15] inclusion of the NLO matrix elements into parton shower Monte Carlo programs. For more details we refer to the individual contributions in these proceedings.

A prioritized list of NLO (and some NNLO) cross sections was assembled at Les Houches in 2005 [16] and added to in 2007 [17] and 2009 [18]. This list includes cross sections which are experimentally important, and which are theoretically feasible (if difficult) to calculate. As we stand now, basically all NLO $2 \rightarrow 3$ and $2 \rightarrow 4$ cross sections of interest have been calculated, see Tables 12 below, and even some processes which were not on the 2009 wishlist are available at NLO, see e.g. [19, 20, 21, 22, 23, 24, 25]. The success of automation techniques means that future NLO calculations of similar complexity can be completed without the man-years of labor previously required. Thus, we do not add to the NLO wish list in 2011. Instead, we comment on calculations needed at NNLO, and processes at NLO for which it is important to calculate the impact of electroweak corrections, and/or the
influence of interference effects with other processes with the same final state.
For many of the processes calculated at the LHC (such as for Higgs production), it is important either to apply a veto for the production of extra jets, or to bin the analysis results according to the jet multiplicity. While such cuts are useful for dealing with the experimental backgrounds, the exclusivity of the cross sections results in increases to the theoretical uncertainties obtained for the corresponding inclusive results, see e.g. [26]. The impact of such cuts is explored in the contribution of Stewart and Tackmann in these proceedings.

Much of the complexity for multi-parton NLO processes consists of the calculation of the nonleading color contributions. Such contributions typically contribute only at the level of a few percent and approximations to the non-leading color contributions should be accurate within a percent or so [70, 71, [51]. So it may be more time-prudent for groups carrying out such calculations to estimate the non-leading color effects before carrying out the full calculation.

To reach full utility, the codes for any of these complex NLO calculations should be made public and/or the authors should generate ROOT ntuples providing the parton level event information from which experimentalists can assemble any cross sections of interest. Where possible, decays (with spin correlations) should be included. A ROOT output option is especially useful where the creation of a user-friendly NLO program may be very time-consuming. We now have some experience with the use of ROOT ntuples with both MCFM and Blackhat+Sherpa calculations. The latter, in particular, does not exist as a public program, while ROOT tuples have been made available for NLO W/Z +n jet multiplicities (with $n$ up to 4 ) for $W / Z+$ jets, and (also for $n$ up to 4 ) for inclusive jet production. The estimation of the correct scale for use in multi-parton NLO calculations, and the proper evaluation of the uncertainty on this scale, is more complex than for simpler calculations. The use of ROOT ntuples can make these evaluations easier to carry out. A contribution describing their use has been included in these proceedings.

While NLO is sufficient for most predictions, it is also crucial to understand certain critical cross sections at NNLO. To date, NNLO calculations have been carried out primarily for processes in $e^{+} e^{-}$ annihilation [72, 73, 74], and in hadronic collisions for $2 \rightarrow 1$ processes, with the exception of VH [75, 76, 77] and $\gamma \gamma$ production [78].

To calculate a $2 \rightarrow 2$ scattering process at NNLO, the divergent contributions arising from the treelevel $2 \rightarrow 4$, the one-loop $2 \rightarrow 3$ and the two-loop $2 \rightarrow 2$ subprocesses have to be properly subtracted and cancelled, such that the finite remainders can be combined into a parton-level event generator. To combine the three contributions, an infra-red subtraction scheme for unresolved real radiation is required. Several approaches have been used and are being further developed: antenna subtraction [79], which currently is extended to hadronic and semi-hadronic initial states [80, 81, 82, 83, 84], a method based on sector decomposition appplied to real radiation [85, 86, 87] where the decomposition is guided by the physical singularity structure [88, 89], $q_{T}$-subtraction [90], which is very elegant but appplicable only to colourless final states, and the one of [91] described in these proceedings.

Further, two-loop amplitudes are interesting in their own right from a field theory point of view, for example to study asymptotic behaviour, or to gain insights into the all-order infared structure of massless field theories.

Below we construct a table of calculations needed at the LHC, and which are feasible within the next few years. Certainly, results for inclusive cross sections at NNLO will be easier to achieve than differential distributions, but most groups are working towards a partonic Monte Carlo program capable of producing fully differential distributions for measured observables.

- $t \bar{t}$ production:
needed for accurate background estimates, top mass measurement, top quark asymmetry (which is zero at tree level, so NLO is the leading non-vanishing order for this observable, and a discrepancy of theory predictions with Tevatron data needs to be understood). Several groups are already well


Table 1: The updated experimenter's wishlist for LHC processes

| Calculations beyond NLO added in 2007 |  |
| :--- | :--- |
| 13. $g g \rightarrow W^{*} W^{*} \mathcal{O}\left(\alpha^{2} \alpha_{s}^{3}\right)$ | backgrounds to Higgs |
| normalization of a benchmark process |  |
| 14. NNLO $p p \rightarrow t \bar{t}$ |  |
| 15. NNLO to VBF and $Z / \gamma+$ jet |  |
| Calculations including electroweak effects |  |
| 16. NNLO QCD+NLO EW for $W / Z$ | precision calculation of a SM benchmark |
| NLO EW to $W / Z$ | $[65,66$ |
| NLO EW to $W / Z+$ jet |  |
| NLO EW to $W H / Z H$ | $[67,6]$ |
| $[69]$ |  |

Table 2: The updated experimenter's wishlist for LHC processes continued
on the way to complete NNLO results for $t \bar{t}$ production [92, 93, 94, 95].

- $W^{+} W^{-}$production:
importand background to Higgs search. At the LHC, $g g \rightarrow W W$ is the dominant subprocess, but $g g \rightarrow W W$ is a loop-induced process, such that two loops need to be calculated to get a reliable estimate of the cross section. Advances towards the full two-loop result are reported in [96, 97].
- inclusive jet/dijet production:

NNLO parton distribution function (PDF) fits are starting to become the norm for predictions and comparisons at the LHC. Paramount in these global fits is the use of inclusive jet production to tie down the behavior of the gluon distribution, especially at high $x$. However, while the other essential processes used in the global fitting are known to NNLO, the inclusive jet production cross section is only known at NLO. Thus, it is crucial for precision predictions for the LHC for the NNLO corrections for this process to be calculated, and to be available for inclusion in the global PDF fits. First results for the real-virtual and double real corrections to gluon scattering can be found in [98, 99].

- $\mathrm{V}+1$ jet production:
$W / Z / \gamma+$ jet production form the signal channels (and backgrounds) for many key physics processes, for both SM and BSM. In addition, they also serve as calibration tools for the jet energy scale and for the crucial understanding of the missing transverse energy resolution. The two-loop amplitudes for this process are known [100, 101], therefore it can be calculated once the parts involving unresolved real radiation are available.
- $\mathrm{V}+\gamma$ production:
important signal/background processes for Higgs and New Physics searches. The two-loop helicity amplitudes for $q \bar{q} \rightarrow W^{ \pm} \gamma$ and $q \bar{q} \rightarrow Z^{0} \gamma$ recently have become available [102].
- Higgs+1 jet production:

As mentioned previously, events in many of the experimental Higgs analyses are separated by the number of additional jets accompanying the Higgs boson. In many searches, the Higgs +0 jet and Higgs +1 jet bins contribute approximately equally to the sensitivity. It is thus necessary to have the same theoretical accuracy for the Higgs +1 jet cross section as already exists for the inclusive Higgs cross section, i.e. NNLO. The two-Loop QCD Corrections to the Helicity Amplitudes for $H \rightarrow 3$ partons are already available [103].

The contributions in this document are arranged as follows. In section II various developments concerning techniques for NLO and NNLO calculations are described, in particular in view of providing
automated tools for NLO corrections. In section III, issues related to parton distribution functions are discussed. Section IV contains phenomenological studies of observables and uncertainties, based on theory input where higher order corrections obtained by different approaches are available. Section V includes phenomenological studies on the definition of experimental observables and corrections applied to data. Finally Section VI discusses issues related to the tuning of Monte Carlos and standardised Monte Carlo output formats.

## Part II

## NLO AUTOMATION AND (N)NLO TECHNIQUES

## 1. PJFRY - A C++ PACKAGE FOR TENSOR REDUCTION OF ONE-LOOP FEYNMAN INTEGRALS ${ }^{1}$


#### Abstract

The C++ package PJFry 1.0.0 [104, 105] - a one loop tensor integral library is introduced. We use an algebraic approach to tensor reduction. As a result, the tensor integrals are presented in terms of scalar one- to four-point functions, which have to be provided by an external library, e.g. QCDLoop/FF or OneLOop or LoopTools/FF. The reduction is implemented until five-point functions of rank five. A numerical example is shown, including a special treatment for small or vanishing inverse four-point Gram determinants. Future modules of PJFry might cover the treatment of $n$-point functions with $n \geq 6$; the corresponding formulae are worked out. Further, an extremely efficient approach to tensor reduction relies on evaluations of complete contractions of the tensor integrals with external momenta. For this, we worked out an algorithm for the analytical evaluation of sums over products of signed minors with scalar products of chords, i.e. differences of external momenta. As a result, the usual multiple sums over tensor coefficients are replaced for the numerical evaluation by compact combinations of the basic scalar functions.


### 1.1 PJFry

The goal of the C++ package PJFry is a stable and fast open-source implementation of one-loop tensor reduction of Feynman integrals

$$
\begin{equation*}
I_{n}^{\mu_{1} \cdots \mu_{R}}=C(\epsilon) \int \frac{d^{d} k}{i \pi^{d / 2}} \frac{\prod_{r=1}^{R} k^{\mu_{r}}}{\prod_{j=1}^{n}\left(k-q_{j}\right)^{2}-m_{j}^{2}+i \epsilon}, \tag{1}
\end{equation*}
$$

suitable for any physically relevant kinematics ${ }^{2}$ The algorithm was invented in [105]. PJFry performs the reduction of 5 -point 1 -loop tensor integrals up to rank 5 . The 4 - and 3 -point tensor integrals are obtained as a by-product. Main features are:

- Any combination of internal or external masses
- Automatic selection of optimal formula for each coefficient
- Leading ()$_{5}$ are eliminated in the reduction

[^192]- Small ()$_{4}$ are avoided using asymptotic expansions where appropriate
- Cache system for tensor coefficients and signed minors
- Interfaces for C, C++, FORTRAN and Mathematica
- Uses QCDLoop [109, 110] or OneLOop [111] for 4-dim scalar integrals
- Available from the project webpage https://github.com/Vayu/PJFry/ [104, 105]

The installation of PJFry may be performed following the instructions given at the project webpage. The project subdirectories are ./src - the library source code ./mlink - the MathLink interface
./examples - the FORTRAN examples of library use, built with make check
A build on Unix/Linux and similar systems is done in a standard way by sequential performing ./configure, make, make install. See the INSTALL file for a detailed description of the ./configure options.

The functions for tensor coefficients for up to rank $R=5$ pentagon integrals are declared in the Mathematica interface:

```
In:= Names["PJFry`*"]
Out={A0v0, B0v0, B0v1, B0v2, C0v0, C0v1, C0v2, C0v3, \
D0v0, D0v1, D0v2, D0v3, D0v4, E0v0, E0v1, E0v2, \
EOv3, EOv4, EOv5, GetMu2, SetMu2}
```

The C++ and Fortran interface syntax is very close to that of e.g. LoopTools/FF:
E0v3[i,j,k,p1s,p2s,p3s,p4s,p5s,s12,s23,s34,s45,s15,m1s,m2s,m3s,m4s,m5s,ep=0]
where 3
i, $\mathrm{j}, \mathrm{k}$ are indices of the tensor coefficient $(0<i \leq j \leq k<n)$,
$\mathrm{p} 1 \mathrm{~s}, \mathrm{p} 2 \mathrm{~s}, \ldots$ are squared external masses $p_{i}^{2}$,
s12, s23, ... are Mandelstam invariants $\left(p_{i}+p_{j}\right)^{2}$,
$\mathrm{m} 1 \mathrm{~s}, \mathrm{~m} 2 \mathrm{~s}, \ldots$ are squared internal masses $m_{i}^{2}$,
$\mathrm{ep}=0,-1,-2$ selects the coefficient of the $\epsilon$-expansion.
The average evaluation time per phase-space point on a 2 GHz Core 2 laptop for the evaluation of all 81 rank 5 tensor form-factors amounts to 2 ms .

A numerical example is shown, for a configuration as in figure 1, in figures 2 and 3 for a five-point rank $R=4$ tensor coefficient in a region, where one of the 4-point sub-Gram determinants vanishes [at $x=0]$ :
$E_{3333}\left(0,0,-6 \times 10^{4}(x+1), 0,0,10^{4},-3.5 \times 10^{4}, 2 \times 10^{4},-4 \times 10^{4}, 1.5 \times 10^{4}, 0,6550,0,0,8315\right)$
The red curve is produced with standard PJFry, and the blue one with Passarino-Veltman [PV] reduction [112]; we mention that for the case treated here $(x \rightarrow 0)$, the PV reduction is no standard option. Our expansion in terms of higher dimensional scalar 3-point functions in case of vanishing 4-point subGram determinants uses only functions $I_{3}^{d+2 l}$ [105]. These are tensor coefficients of the pure $g^{\mu \nu}$ type [113], and so our method is different from others with a mixed numerical approach [114] or with use of additional tensor coefficients [115].

Tensor reduction by PJFry is used as one option of the GoSam package [12]. An older version of the algorithm, as described in [116], has been implemented independently in [11].

[^193]

Fig. 1: Momenta definitions for PJFry.

### 1.2 POTENTIAL UPGRADES

### 1.21 Tensor reduction for higher-point functions

So far, PJFry is foreseen for 5-point functions and simpler ones. The extension to 6-point functions is known from e.g. [114, 115, [116]. In [107] we solve analytically generalized recursions for $n \geq 6$, derived in [114]:

$$
\begin{equation*}
I_{n}^{\mu_{1} \mu_{2} \ldots \mu_{R}}=-\sum_{r=1}^{n} C_{r}^{\mu_{1}}(n) I_{n-1}^{\mu_{2} \cdots \mu_{R}, r} \tag{2}
\end{equation*}
$$

where in $I_{n-1}^{\mu, \cdots, r}$ the line $r$ is scratched. The coefficients for 6-point functions are:

$$
\begin{equation*}
C_{r}^{s, \mu}(6)=\sum_{i=1}^{5} \frac{1}{\binom{0}{s}_{6}}\binom{0 r}{s i}_{6} q_{i}^{\mu_{1}}, s=0 \ldots 6, \tag{3}
\end{equation*}
$$

where the $q_{i}$ are chords, and $\binom{0 r}{s i}_{6}$ etc. are signed minors with arbitrary $s$. For the 7-point and 8-point functions, we found several representations, among them

$$
\begin{equation*}
C_{r}^{s t, \mu}(7)=\sum_{i=1}^{6} \frac{1}{\binom{(t)^{2}}{s t}_{7}}\binom{s t i}{s t r}_{7} q_{i}^{\mu} \tag{4}
\end{equation*}
$$

and

$$
\begin{equation*}
C_{r}^{s t u, \mu}(8)=\sum_{i=1}^{7} \frac{1}{\binom{s t u}{s t u}_{8}}\binom{\text { stui }}{\text { stur }}_{8} q_{i}^{\mu} \tag{5}
\end{equation*}
$$

The upper indices $s, t$ and $u$ stand for the redundancy of the solutions and can be freely chosen.

### 1.22 Evaluation of contracted tensor integrals using sums over signed minors

The contraction of a tensor integral with chords may be written as a sum over basic scalar integrals (at a stage where they are free of tensor coefficient indices), multiplied by (multiple) sums over chords times


Fig. 2: Absolute accuracy of $E_{3333}$ in the region of vanishing sub-Gram determinant. Blue curve: conventional Passarino-Veltman reduction, red curve: PJFry.
signed minors. If one may perform these sums algebraically, the method becomes very efficient. And this has been systematically worked out in [106], see also [108].

We reproduce here two 7-point examples.
The rank $R=2,3$ integrals become by contraction

$$
\begin{align*}
q_{a, \mu} q_{b, \nu} I_{7}^{\mu \nu} & =\sum_{r, t=1}^{7} K^{a b, r t} I_{5}^{r t},  \tag{6}\\
q_{a, \mu} q_{b, \nu} q_{c, \lambda} I_{7}^{\mu \nu \lambda} & =\sum_{r, t, u=1}^{7} K^{a b c, r t u} I_{4}^{r t u}, \tag{7}
\end{align*}
$$

where $I_{5}^{r t}$ and $I_{4}^{r t u}$ are scalar 5- and 4-point functions, arising from the 7-point function by scratching lines $r, t, \ldots$ In the general case, we have at this stage higher-dimensional integrals $I_{n}^{d+2 l}, n=2, \ldots, 5$, to be further reduced following the known scheme, if needed. Here, the $I_{5}^{r t}$ have to be expressed by 4 -point functions.

The expansion coefficients are factorizing here,

$$
\begin{align*}
K^{a b, r t} & =K^{a, r} K^{b, r t},  \tag{8}\\
K^{a b c, r t u} & =-K^{a, r} K^{b, r t} K^{c, r t u} \tag{9}
\end{align*}
$$

and the sums over signed minors have been performed analytically:

$$
\begin{gather*}
K^{a, r}=\frac{1}{2}\left(\delta_{a r}-\delta_{7 r}\right),  \tag{10}\\
K^{b, r t}=\sum_{j=1}^{6}\left(q_{b} q_{j}\right) \frac{\left(\begin{array}{c}
r s t \\
r s)_{7}
\end{array}\right.}{\binom{r s}{r s}_{7}} \equiv \frac{\Sigma_{b}^{1, s t u}}{\binom{r s}{r s}_{7}}=\frac{1}{2}\left(\delta_{b t}-\delta_{7 t}\right)-\frac{1}{2} \frac{\binom{r s}{t s}_{7}}{\binom{r s}{r s}}\left(\delta_{b r}-\delta_{7 r}\right), \tag{11}
\end{gather*}
$$



Fig. 3: Relative accuracy of $E_{3333}$ in the region of vanishing sub-Gram determinant. At $x \sim 0.0015$, PJFry switched to the asymptotic expansion.

$$
\begin{align*}
K^{a, s t u} & =\sum_{i=1}^{6}\left(q_{a} q_{i}\right)\binom{0 s t u}{0 s t i}_{7} \equiv \Sigma_{a}^{2, s t u}  \tag{12}\\
& =\frac{1}{2}\left\{\binom{s t u}{s t 0}_{7}\left(Y_{a 7}-Y_{77}\right)+\binom{0 s t}{0 s t}_{7}\left(\delta_{a u}-\delta_{7 u}\right)-\binom{0 s t}{0 s u}_{7}\left(\delta_{a t}-\delta_{7 t}\right)-\binom{0 t s}{0 t u}_{7}\left(\delta_{a s}-\delta_{7 s}\right)\right\}
\end{align*}
$$

with

$$
\begin{equation*}
Y_{j k}=-\left(q_{j}-q_{k}\right)^{2}+m_{j}^{2}+m_{k}^{2} \tag{13}
\end{equation*}
$$

Conventionally, $q_{7}=0$.
The sums may be found in eqns. (A.15) and (A.16) of [106]. The $s$ is redundant and fulfils $s \neq r, b, 7$ in $K^{b, r t}$. In $K_{0}^{a, s t u}$ it is $s, t, u=1, \ldots 7$ with $s \neq u, t \neq u$.

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## 2. THE GOSAM APPROACH TO AUTOMATED ONE-LOOP CALCULATIONS ${ }^{4}$


#### Abstract

We describe the GoSAM framework for the automated computation of multiparticle scattering amplitudes at the one-loop level. The amplitudes are generated explicitly in terms of Feynman diagrams, and can be evaluated using either $d$-dimensional reduction at the integrand level or tensor decomposition. GoSAM can be used to compute one-loop QCD and EW corrections to Standard Model processes, and it is ready to link generic model files for theories Beyond the Standard Model.


[^194]
### 2.1 Introduction and General Motivations

In the last few years we observed major advances in the direction of constructing packages for fully automated one-loop calculations, which profited from the new developments in the field of NLO QCD calculations [17, 18]. The continuous improvement of the techniques for one-loop computations led to important new results for processes with many particles [51, 70, 117, 71, 53, 48, 49, 50, 54, 62, 63, 23, 118, 25, 56, 57, 21, 22, 20, 19].

Very advanced calculations have been performed with improved algebraic reduction methods based on Feynman-diagrammatic algorithms, as well as with new numerical techniques based on the idea of reconstructing one-loop amplitudes from their unitarity cuts. These theoretical developments found an ideal counterpart in the integrand-level reduction algorithm, that allows for the reduction of any scattering amplitudes to scalar master integrals, simply by evaluating numerically the integrand at given fixed values of the integration momentum. In both scenarios, to tackle the increase in the complexity and in the number of diagrams that contribute to the amplitudes, automation becomes indispensable for processes with many external legs.

The purpose of the present document is to illustrate the main features of GoSam [12], a new framework which allows the automated calculation of one-loop scattering amplitudes for multi-particle processes. This approach combines the automated algebraic generation of $d$-dimensional unintegrated amplitudes obtained via Feynman diagrams, with the numerical integrand-level reduction provided by the $d$-dimensional extension [119, 120, 6] of the OPP integrand-level reduction method [121, 122, 123] and improved tensorial techniques [124, 125].

The integrands of the one-loop amplitudes are generated via Feynman diagrams, using QGRAF [126], FORM [127], spinney [128] and haggies [129]. The only task required from the user is the preparation of an "input card" to start the generation of the source code and its compilation, without having to worry about internal details of the code generation. The individual program tasks are efficiently managed by python scripts. Concerning the reduction, the program offers the possibility to use either the $d$-dimensional extension of the OPP method, as implemented in SAMURAI [6], or tensor reduction as implemented in Golem95C [130, 131] interfaced through tensorial reconstruction at the integrand level [124].

### 2.2 Algebraic approach to Automation

There are several approaches to the automated computation of multi-particle scattering amplitudes at the one-loop level, which provide different recipes for the construction of multi-purpose tools. The goal of such tools is the evaluation of one-loop scattering amplitudes for any choice of particles in the initial and final states, in a fully automated manner.

In the algebraic approach to multi-purpose automation, amplitudes can be generated from Feynman diagrams by employing tools for algebraic manipulation: already some time ago, the idea of automating NLO calculations has been pursued by public programs like FeynArts [132] and QGRAF [126] for diagram generation and FormCalc/LoopTools [133] and GRACE [3] for the automated calculation of NLO corrections, primarily in the electroweak sector.

When we combine the algebraic generation with the integrand-level reduction, the set of algebraic operations required are quite different with respect to a traditional tensorial reduction. Since the target is to provide the numerical value of the numerator function at given values of integration momentum, we should aim at expressions for the unintegrated numerator that are easily evaluated numerically. To achieve this task, for example, expressions in terms of spinor products are particularly convenient.

We briefly list here some of the advantages of the "algebraic approach": i) the algebraic generation is executed separately from the numerical reduction, therefore algebraic manipulations are possible before starting the numerical integration; CPU-time can be spent, once for all at the beginning of the calculation, to optimize and reduce the size of the integrands that will be evaluated numerically several times
later on during the reduction; ii) the algebraic method allows us to group sets of diagrams and cache all factors that do not depend on the integration momentum; iii) easy access to sub-parts of the computation; subsets of diagrams can be easily added or removed from the final results, simplifying comparisons and tests; iv) computer algebra can be performed in dimension $d$ using alternative regularization schemes; v) the choice between different reduction algorithms can be performed at run-time, providing flexibility and internal cross-checks. In the next section we will briefly illustrate how these properties are used within GoSAM.

Important progress in a similar direction has been also recently achieved by means of FeynArts, FormCalc and LoopTools [134, 2] to provide amplitudes that can be processed using the integrand-level reduction provided by CutTools [135] and/or SAMURAI [6] or with the traditional Passarino-Veltman reduction [112].

### 2.3 A brief introduction to GoSAM

GoSAM produces in a fully automated way all the code required to perform the calculation of virtual one-loop amplitudes. The only task left to the user is the preparation of an "input card" which contains all the information related to the particular process namely initial and final particles, model, helicities, selection rules to exclude particular sets of diagrams, regularization scheme. The card also contains flags to select the preferred reduction methods and some optimization flags to adapt the diagram generation to the needs of the user.

There are three main steps that GoSAM follows in order to prepare the code for the calculation: the generation of diagrams that contribute to the process, the optimization and algebraic manipulation to simplify their expressions, and the writing of a FORTRAN code ready to be used within a phase-space integration. It is important to remember that these steps will only be performed once. After the code is generated, the reduction of unintegrated amplitudes to linear combinations of scalar (master) integrals is fully embedded in the process and can be performed with different options, all available at run-time. Only the last part, namely the reduction and evaluation of master integrals, will be repeated for all the different phase-space points that contribute to the cross-section.

### 2.31 Diagram Generation

For the diagram generation both at tree level and one-loop level we employ QGRAF [126] which we complemented by adding another filter over diagrams implemented in Python. This gives several advantages since it increases the ability of the code to distinguish certain classes of diagrams and group them according to the sets of their propagators, in order to fully optimize the reduction.

At this stage GoSAm generates three sets of output files: an expression for each diagram for FORM [127], Python code for drawing each diagram, and Python code for computing the properties of the diagram. Information about the model is either read from the built-in Standard Model of QGRAF or can be defined by the user by means of LanHEP [136] or an Universal FeynRules Output (UFO) file [137]

The Python program automatically performs several operations: diagrams whose color factor turns out to be zero are dropped; the number of propagators containing the loop momentum, the tensor rank and the kinematic invariants of the associated loop integral are computed; diagrams with a vanishing loop integral associated are detected and flagged for the diagram selection; all propagators and vertices are classified for the diagram selection; diagrams containing massive quark self-energy insertions or closed massless quark loops are specially flagged.

During this phase, GoSAM also generates a ETEX file which contains, among other useful information of the generated process, the drawings of all contributing diagrams. To achieve this task, we use our own implementation of the algorithms described in Ref. [138] and Axodraw [139] to actually draw the diagrams.

### 2.32 Lorentz Algebra

Concerning the algebraic operations performed by GoSAM to render the integral suitable for efficient numerical evaluation, one of the primary goals is to split the $(4-2 \varepsilon)$ dimensional algebra into strictly four-dimensional objects and symbols representing the higher-dimensional remainder. All external vectors (momenta and polarisation vectors) are kept in four dimensions; internal vectors, however, are kept in the $d$-dimensional vector space.

We adopt the conventions used in [128], where $\hat{k}$ denotes the four dimensional projection of an in general $d$ dimensional vector $k$. The $(d-4)$ dimensional orthogonal projection is denoted as $\tilde{k}$. For the integration momentum $q$ we introduce in addition the symbol $\mu^{2}=-\tilde{q}^{2}$, such that

$$
\begin{equation*}
q^{2}=\hat{q}^{2}+\tilde{q}^{2}=\hat{q}^{2}-\mu^{2} . \tag{14}
\end{equation*}
$$

We also introduce suitable projectors by splitting the metric tensor

$$
\begin{equation*}
g^{\mu \nu}=\hat{g}^{\mu \nu}+\tilde{g}^{\mu \nu}, \quad \hat{g}^{\mu \nu} \tilde{g}_{\nu \rho}=0, \quad \hat{g}_{\mu}^{\mu}=4, \quad \tilde{g}_{\mu}^{\mu}=d-4 \tag{15}
\end{equation*}
$$

Once all propagators and all vertices have been replaced by their corresponding expressions, according to the model file, all vector-like quantities and metric tensors are split into their four-dimensional and their orthogonal part. As we use the 't Hooft algebra, $\gamma_{5}$ is defined as a purely four-dimensional object, $\gamma_{5}=i \epsilon_{\mu \nu \rho \sigma} \hat{\gamma}^{\mu} \hat{\gamma}^{\nu} \hat{\gamma}^{\rho} \hat{\gamma}^{\sigma}$. By applying the usual anti-commutation relation for Dirac matrices we can always separate the four-dimensional and $(d-4)$-dimensional parts of Dirac traces.

While the $(d-4)$-dimensional traces are reduced completely to products of $(d-4)$-dimensional metric tensors, the four-dimensional part, which will be reduced numerically, is treated such that the number of terms in the resulting expression is kept as small as possible.

### 2.33 Treatment of rational terms $R_{2}$

Instead of relying on the construction of $R_{2}$ from specialized Feynman rules [123, 140, 141, 142, 143], we can generate the $R_{2}$ part along with all other contribution using automated algebraic manipulations. The code offers the option between the implicit and explicit construction of the $R_{2}$ terms. The implicit construction treats the $4-$ and $(d-4)$ dimensional numerators on equal grounds: they are generated algebraically and reduced numerically. The explicit construction of $R_{2}$ is based on the fact that the $(d-4)$ dimensional part of the numerator function contains expressions for the corresponding integrals that are relatively simple and known explicitly. Therefore, after separating it using the algebraic manipulation described before, the $(d-4)$ dimensional part is computed analytically whereas the purely four-dimensional part is passed to the numerical reduction. This approach also allows for an efficient calculation of the part $R_{2}$ alone.

### 2.34 Reduction to scalar (master) integrals

GoSAM allows to choose at run-time (i.e. without re-generating the code) the preferred method of reduction. Available options include the integral-level $d$-dimensional reduction, as implemented in SAMURAI, or traditional tensor reduction as implemented in Golem95C interfaced through tensorial reconstruction at the integrand level, or a combination of both. Concerning the scalar (tensorial) integrals, GoSAM allows to choose among a variety of options, including QCDLoop [109], OneLoop [111], Golem95C [130], plus the recently added P JFRY [108]. Among these codes, OneLoop and Golem95C also fully support complex masses.

### 2.4 Installation and Usage

GoSam can be used within a standard Linux/Unix environment. In order to work, it requires some programs to be installed on the system: these include a recent version of Python (version $\geq 2.6$ ), Java
( $\geq 1.5$ ), a Fortran 95 compiler, FORM (version $\geq 3.3$ ), and QGRAF. Further, at least one of the libraries SAMURAI or Golem95C needs to be present at the time the code is compiled.

To facilitate this task, we have prepared a package containing SAMURAI and Golem95C together with the libraries for the integrals: OneLOop, QCDLoop, and FF. The package, which is called gosam-contrib-1.0.tar.gz is available for download from

```
http://projects.hepforge.org/gosam/.
```

The installation procedure is facilitated by the use of Autotools.
The user can download the GoSAM code either as a tar-ball or from the subversion repository at http://projects.hepforge.org/gosam/. The installation of GoSam is controlled by Python Distutils and can be performed by simply running the command

```
python setup.py install
```

In order to generate the code for a process, the user needs to prepare an input file (process card) which contains:

- process specific information, such as a list of initial and final state particles, their helicities (optional) and the order of the coupling constants;
- scheme specific information, such as the regularisation and renormalisation schemes, the underlying model, masses and widths which are set to zero;
- system specific information, such as paths to programs and libraries or compiler options;
- optional information for optimisations within the code generation.

Assuming that the process card is called myprocess.in, the generation of the code can be started by simply running the command gosam.py myprocess.in. All further steps are controlled by makefiles which are automatically generated by GoSAM: the command make compile generates the source code and compiles all files relevant for the production of the matrix element. The code can be tested with the program test. f 90 (located in the subdirectory matrix) which provides, for a random phase-space point, the tree-level LO matrix element and the NLO result for the finite part, single and double poles. Examples of process cards for a selection of benchmark processes are provided with the main distubution.

For more details about the usage and installation of GoSAM, we refer the user to a more technical presentation [144] or to the original publication [12] and the user manual which accompanies the code.

### 2.5 Examples of Applications

The BLHA interface [145] allows to link GoSAM to a general Monte Carlo event generator, which is responsible for supplying the missing ingredients for a complete NLO calculation of a physical cross section. Among those, SHERPA [146] offers the possibility to compute the LO cross section and the real corrections with both the subtraction terms and the corresponding integrated counterparts [147]. Using the BLHA interface, we linked GoSAM with SHERPA to compute the physical cross section for $W^{ \pm}+1$-jet at NLO, which is described in Section 18 .

The codes produced by GoSam have been tested on several processes of increasing complexity, some of which are shown in Table 1. The full list of processes produced by GoSam and compared to the literature where available is given in Ref. [12].

As an example of the usage of GoSam with a model file different from the Standard Model, we calculated the QCD corrections to neutralino pair production in the MSSM. The model file has been imported using the UFO interface. In this calculation, we combined the one-loop amplitude with the real radiation corrections to obtain results for differential cross sections. For the infrared subtraction terms

| $e^{+} e^{-} \rightarrow u \bar{u}$ | $[148]$ |
| :--- | :--- |
| $e^{+} e^{-} \rightarrow t \bar{t}$ | $[149,150]$, own analytic calculation |
| $u \bar{u} \rightarrow d \bar{d}$ | $[15$, 8] |
| $g g \rightarrow g g$ | $[152]$ |
| $g g \rightarrow g Z$ | $[153]$ |
| $b g \rightarrow H b$ | $[154,8]$ |
| $\gamma \gamma \rightarrow \gamma \gamma(\mathrm{W}$ loop) | $[15]$ |
| $\gamma \gamma \rightarrow \gamma \gamma \gamma \gamma$ (fermion loop) | $[156]$ |
| $p p \rightarrow t \bar{t}$ | $[8]$, MCFM [157, 158] |
| $p p \rightarrow W^{ \pm} j$ (QCD corr.) | $[157,158]$ |
| $p p \rightarrow W^{ \pm} j$ (EW corr.) | for IR poles: [65, 159] |
| $p p \rightarrow W^{ \pm} t$ | $[157,158]$ |
| $p p \rightarrow W^{ \pm} j j$ | $[157,158]$ |
| $p p \rightarrow W^{ \pm} b \bar{b}$ (massive b) | $[157,158$ |
| $e^{+} e^{-} \rightarrow e^{+} e^{-} \gamma(\mathrm{QED})$ | $[160]$ |
| $p p \rightarrow H t t \bar{t}$ | $[8]$ |
| $p p \rightarrow Z t \bar{t}$ | $[10]$ |
| $p p \rightarrow W^{+} W^{+} j j$ | $[56$, v3] |
| $p p \rightarrow b \bar{b} b \bar{b}$ | $[62,63]$ |
| $p p \rightarrow W^{+} W^{-} b \bar{b}$ | $[8,161]$ |
| $p p \rightarrow t \bar{t} b \bar{b}$ | $[8,161]$ |
| $u \bar{d} \rightarrow W^{+} g g g$ | $[161]$ |

Table 3: Some of the processes computed and checked with GoSAm
we employed MadDipole [162], while the real emission part is calculated using MadGraph/MadEvent [163]. The virtual matrix element is renormalized in the $\overline{M S}$ scheme, while massive particles are treated in the on-shell scheme. The renormalization terms specific to the massive MSSM particles have been added manually. In Fig $\sqrt[4]{ }$ we show the differential cross section for the $m_{\chi_{1}^{0} \chi_{1}^{0}}$ invariant mass, where we employed a jet veto to suppress large contributions from the channel $q g \rightarrow \chi_{1}^{0} \chi_{1}^{0} q$ which opens up at order $\alpha^{2} \alpha_{s}$, but for large $p_{T}^{j e t}$ belongs to the distinct process of neutralino pair plus one hard jet production at leading order.


Fig. 4: Comparison of the NLO and LO $m_{\chi_{1}^{0} \chi_{1}^{0}}$ distributions for the process $p p \rightarrow \chi_{1}^{0} \chi_{1}^{0}$ with a jet veto on jets with $p_{T}^{j e t}>20 \mathrm{GeV}$ and $\eta<4.5$. The band gives the dependence of the result on $\mu=\mu_{F}=\mu_{R}$ between $\mu_{0} / 2$ and $2 \mu_{0}$. We choose $\mu_{0}=m_{Z}$.

## Conclusions and Outlook

Several groups are currently working at the development of automated multi-purpose tools for one-loop calculations. For quite a long time, tree-level calculation have been fully automated and included in flexible multi-process tools [164, 165]. The level of automation achieved by one-loop calculations is suggesting the possibility of a similar success also at the next-lo-leading order. The target is to build efficient and flexible NLO programs which can be used to tackle the increasing need of precision required by the experimental collaborations.

GoSam is a flexible and broadly applicable tool for the fully automated evaluation of one-loop scattering amplitudes. In this approach, scattering amplitudes are generated in terms of Feynman diagrams and their reduction to master integrals can be performed in several ways, which can be selected at run-time. GoSAm can be used to calculate one-loop corrections both in QCD and electro-weak theory and offers the flexibility to link general model files for theories Beyond the Standard Model. The code performed well in reproducing a wide range of examples and we are looking forward to tackle more challenging calculations and interfacing with other existing tools in the near future.

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## 3. AUTOMATION AND NUMERICAL LOOP INTEGRATION ${ }^{5}$

### 3.1 INTRODUCTION

Numerical methods are nowadays routinely used in fully differential fixed-order perturbative calculations for the integration over the phase-space of the final-state particles. The use of numerical methods for the phase-space integration allows the flexibility to compute any infrared-safe observable for a given process within a single numerical program. It is thus natural to investigate if numerical methods can also be applied for the loop integration in the virtual corrections [166, 167, $168,169,170,171,172,173$ [174, 175, 176]. A major breakthrough was achieved recently by showing that the numerical method is compatible in efficency with the commonly used approaches based on cut techniques and generalised unitarity or on Feynman graphs [70, [51, 53, 22, 20, 52, 117, 56, 54, 50, 48, 177, 111, 5, 178, 8, 12]. The implementation of the numerical method for the loop integration is process-independent and offers therefore the flexibility to compute several processes within one numerical program. We discuss the main principles of the numerical method for the loop integration at one-loop. In addition we give an outlook towards higher loops.

### 3.2 THE SUBTRACTION METHOD FOR THE LOOP INTEGRATION

The contributions to an infrared-safe $n$-jet observable observable $O$ at next-to-leading order are given by

$$
\begin{equation*}
\langle O\rangle^{N L O}=\int_{n+1} O_{n+1} d \sigma^{R}+\int_{n} O_{n} d \sigma^{V}+\int_{n} O_{n} d \sigma^{C} . \tag{16}
\end{equation*}
$$

[^195]Here a rather condensed notation is used. $d \sigma^{R}$ denotes the real emission contribution, whose matrix elements are given by the square of the Born amplitudes with $(n+3)$ partons $\left|A_{n+3}^{(0)}\right|^{2} . d \sigma^{V}$ denotes the virtual contribution, whose matrix elements are given by the interference term of the one-loop and Born amplitude $\operatorname{Re}\left(A_{n+2}^{(0)^{*}} A_{n+2}^{(1)}\right)$ and $d \sigma^{C}$ denotes a collinear subtraction term, which subtracts the initial state collinear singularities. Each term is separately divergent and only their sum is finite.

The subtraction method is widely used to render the real emission part of a NLO calculation suitable for a numerical Monte Carlo integration. One adds and subtracts a suitably chosen piece to be able to perform the phase-space integrations by Monte Carlo methods:

$$
\begin{equation*}
\langle O\rangle^{N L O}=\int_{n+1}\left(O_{n+1} d \sigma^{R}-O_{n} d \sigma^{A}\right)+\int_{n}\left(O_{n} d \sigma^{V}+O_{n} d \sigma^{C}+O_{n} \int_{1} d \sigma^{A}\right) . \tag{17}
\end{equation*}
$$

The first term $\left(O_{n+1} d \sigma^{R}-O_{n} d \sigma^{A}\right)$ is by construction integrable over the $(n+1)$-particle phase-space and can be evaluated numerically. The result of the integration of the subtraction term over the unresolved one-parton phase-space is written in a compact notation as

$$
\begin{equation*}
d \sigma^{C}+\int_{1} d \sigma^{A}=(\mathbf{I}+\mathbf{K}+\mathbf{P}) \otimes d \sigma^{B} \tag{18}
\end{equation*}
$$

The notation $\otimes$ indicates that colour correlations due to the colour charge operators $\mathbf{T}_{i}$ still remain. The terms with the insertion operators $\mathbf{K}$ and $\mathbf{P}$ pose no problem for a numerical evaluation. The term $\mathbf{I} \otimes d \sigma^{B}$ lives on the phase-space of the $n$-parton configuration and has the appropriate singularity structure to cancel the infrared divergences coming from the one-loop amplitude. Therefore $d \sigma^{V}+\mathbf{I} \otimes d \sigma^{B}$ is infrared finite.

We extend this subtraction method to the virtual part such that we can evaluate the one-loop integral of the one-loop amplitude numerically. The renormalised one-loop amplitude $\mathcal{A}^{(1)}$ is related to the bare amplitude $\mathcal{A}_{\text {bare }}^{(1)}$ by $\mathcal{A}^{(1)}=\mathcal{A}_{\mathrm{bare}}^{(1)}+\mathcal{A}_{\mathrm{CT}}^{(1)}$, where $\mathcal{A}_{\mathrm{CT}}^{(1)}$ denotes the ultraviolet counterterm from renormalisation. The bare amplitude involves the loop integration

$$
\begin{equation*}
\mathcal{A}_{\mathrm{bare}}^{(1)}=\int \frac{d^{D} k}{(2 \pi)^{D}} \mathcal{G}_{\mathrm{bare}}^{(1)} . \tag{19}
\end{equation*}
$$

where $\mathcal{G}_{\text {bare }}^{(1)}$ denotes the integrand of the bare one-loop amplitude. We introduce subtraction terms which match locally the singular behaviour of the bare integrand:

$$
\begin{equation*}
\mathcal{A}_{\text {bare }}^{(1)}+\mathcal{A}_{\mathrm{CT}}^{(1)}=\int \frac{d^{D} k}{(2 \pi)^{D}}\left(\mathcal{G}_{\text {bare }}^{(1)}-\mathcal{G}_{\mathrm{soft}}^{(1)}-\mathcal{G}_{\mathrm{coll}}^{(1)}-\mathcal{G}_{\mathrm{UV}}^{(1)}\right)+\left(\mathcal{A}_{\mathrm{CT}}^{(1)}+\mathcal{A}_{\mathrm{soft}}^{(1)}+\mathcal{A}_{\text {coll }}^{(1)}+\mathcal{A}_{\mathrm{UV}}^{(1)}\right) . \tag{20}
\end{equation*}
$$

Analogous to $\mathcal{G}_{\text {bare }}^{(1)}$, the integrands of the subtraction terms $\mathcal{A}_{x}^{(1)}$ are denoted by $\mathcal{G}_{x}^{(1)}$, where $x$ is equal to soft, coll or UV. The expression in the first bracket is finite and can therefore be integrated numerically in four dimensions. The integrated subtraction terms in the second bracket are easily calculated analytically in $D$ dimensions. The result can be written as

$$
\begin{equation*}
2 \operatorname{Re} \mathcal{A}^{(0)}\left(\mathcal{A}_{\mathrm{CT}}^{(1)}+\mathcal{A}_{\mathrm{soft}}^{(1)}+\mathcal{A}_{\mathrm{coll}}^{(1)}+\mathcal{A}_{\mathrm{UV}}^{(1)}\right)^{*} O_{n} d \phi_{n}=\mathbf{L} \otimes d \sigma^{B} . \tag{21}
\end{equation*}
$$

The insertion operator $\mathbf{L}$ contains the explicit poles in the dimensional regularisation parameter related to the infrared singularities of the one-loop amplitude. These poles cancel when combined with the insertion operator $\mathbf{I}$ :

$$
\begin{equation*}
(\mathbf{I}+\mathbf{L}) \otimes d \sigma^{B}=\text { finite } \tag{22}
\end{equation*}
$$

The operator $\mathbf{L}$ contains, as does the operator $\mathbf{I}$, colour correlations due to soft gluons. In analogy to the one-loop amplitude we can write $d \sigma^{V}=d \sigma_{\mathrm{CT}}+\int \frac{d^{D} k}{(2 \pi)^{D}} d \sigma_{\text {bare }}^{V}$ and then the NLO contributions reads

$$
\begin{align*}
& \langle O\rangle^{N L O}=  \tag{23}\\
& \quad \int_{n+1}\left(O_{n+1} d \sigma^{R}-O_{n} d \sigma^{A}\right)+\int_{n+\text { loop }} O_{n}\left(d \sigma_{\text {bare }}^{V}-d \sigma^{A^{\prime}}\right)+\int_{n} O_{n}(\mathbf{I}+\mathbf{L}+\mathbf{K}+\mathbf{P}) \otimes d \sigma^{B} .
\end{align*}
$$

In a condensed notation this reads

$$
\begin{equation*}
\langle O\rangle^{N L O}=\langle O\rangle_{\text {real }}^{N L O}+\langle O\rangle_{\text {virtual }}^{N L O}+\langle O\rangle_{\text {insertion }}^{N L O} . \tag{24}
\end{equation*}
$$

Every single term is finite and can be evaluated numerically.

### 3.3 THE SUBTRACTION TERMS

Amplitudes in QCD may be decomposed into group-theoretical factors (carrying the colour structures) multiplied by kinematic factors called partial amplitudes. At the loop level partial amplitudes may further be decomposed into primitive amplitudes. It is simpler to work with primitive one-loop amplitudes instead of a full one-loop amplitude. Our method exploits the fact that primitive one-loop amplitudes have a fixed cyclic ordering of the external legs and that they are gauge-invariant. The first point ensures that there are at maximum $n$ different loop propagators in the problem, where $n$ is the number of external legs, while the second property of gauge invariance is crucial for the proof of the method. We therefore consider in the following just a single primitive one-loop amplitude, which we denote by $A^{(1)}$, while keeping in mind that the full one-loop amplitude is just the sum of several primitive amplitudes multiplied by colour structures. We label the external momenta clockwise by $p_{1}, p_{2}, \ldots, p_{n}$ and define $q_{i}=p_{1}+$ $p_{2}+\ldots+p_{i}, k_{i}=k-q_{i}$. We can write the bare primitive one-loop amplitude in Feynman gauge as

$$
\begin{equation*}
A_{\text {bare }}^{(1)}=\int \frac{d^{D} k}{(2 \pi)^{D}} G_{\text {bare }}^{(1)}, \quad G_{\text {bare }}^{(1)}=P(k) \prod_{i=1}^{n} \frac{1}{k_{i}^{2}-m_{i}^{2}+i \delta} . \tag{25}
\end{equation*}
$$

$G_{b a r e}^{(1)}$ is the integrand of the bare one-loop amplitude. $P(k)$ is a polynomial in the loop momentum $k$. The $+i \delta$-prescription instructs us to deform - if possible - the integration contour into the complex plane to avoid the poles at $k_{i}^{2}=m_{i}^{2}$. If a deformation close to a pole is not possible, we say that the contour is pinched. If we restrict ourselves to non-exceptional external momenta, then the divergences of the one-loop amplitude related to a pinched contour are either due to soft or collinear partons in the loop. These divergences are regulated within dimensional regularisation by setting the number of space-time dimensions equal to $D=4-2 \varepsilon$. A primitive amplitude which has soft or collinear divergences must have at least one loop propagator which corresponds to a gluon. An amplitude which just consists of a closed fermion loop does not have any infrared divergences. We denote by $I_{g}$ the set of indices $i$, for which the propagator $i$ in the loop corresponds to a gluon. The soft and collinear subtraction terms for massless QCD read [169]

$$
\begin{align*}
G_{\mathrm{soft}}^{(1)} & =16 \pi \alpha_{s} i \sum_{j \in I_{g}} \frac{p_{j} \cdot p_{j+1}}{k_{j-1}^{2} k_{j}^{2} k_{j+1}^{2}} A_{j}^{(0)}, \\
G_{\mathrm{coll}}^{(1)} & =-8 \pi \alpha_{s} i \sum_{j \in I_{g}}\left[\frac{S_{j} g_{\mathrm{UV}}\left(k_{j-1}^{2}, k_{j}^{2}\right)}{k_{j-1}^{2} k_{j}^{2}}+\frac{S_{j+1} g_{\mathrm{UV}}\left(k_{j}^{2}, k_{j+1}^{2}\right)}{k_{j}^{2} k_{j+1}^{2}}\right] A_{j}^{(0)}, \tag{26}
\end{align*}
$$

where $S_{j}=1$ if the external line $j$ corresponds to a quark and $S_{j}=1 / 2$ if it corresponds to a gluon. The function $g_{\mathrm{UV}}$ ensures that the integration over the loop momentum is ultraviolet finite. Integrating
the soft and the collinear part we obtain

$$
\begin{align*}
& S_{\varepsilon}^{-1} \mu_{s}^{2 \varepsilon} \int \frac{d^{D} k}{(2 \pi)^{D}} G_{\mathrm{soft}}^{(1)}=-\frac{\alpha_{s}}{4 \pi} \frac{e^{\varepsilon \gamma_{E}}}{\Gamma(1-\varepsilon)} \sum_{j \in I_{g}} \frac{2}{\varepsilon^{2}}\left(\frac{-2 p_{j} p_{j+1}}{\mu_{s}^{2}}\right)^{-\varepsilon} A_{j}^{(0)}+\mathcal{O}(\varepsilon) \\
& S_{\varepsilon}^{-1} \mu_{s}^{2 \varepsilon} \int \frac{d^{D} k}{(2 \pi)^{D}} G_{\mathrm{coll}}^{(1)}=-\frac{\alpha_{s}}{4 \pi} \frac{e^{\varepsilon \gamma_{E}}}{\Gamma(1-\varepsilon)} \sum_{j \in I_{g}}\left(S_{j}+S_{j+1}\right) \frac{2}{\varepsilon}\left(\frac{\mu_{u v}^{2}}{\mu_{s}^{2}}\right)^{-\varepsilon} A_{j}^{(0)}+\mathcal{O}(\varepsilon) \tag{27}
\end{align*}
$$

$S_{\varepsilon}=(4 \pi)^{\varepsilon} e^{-\varepsilon \gamma_{E}}$ is the typical volume factor of dimensional regularisation, $\gamma_{E}$ is Euler's constant and $\mu$ is the renormalisation scale.

The ultraviolet subtraction terms correspond to propagator and vertex corrections. The subtraction terms are obtained by expanding the relevant loop propagators around a new ultraviolet propagator $\left(\bar{k}^{2}-\right.$ $\left.\mu_{\mathrm{UV}}^{2}\right)^{-1}$, where $\bar{k}=k-Q$ : For a single propagator we have

$$
\frac{1}{(k-p)^{2}}=\frac{1}{\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}}+\frac{2 \bar{k} \cdot(p-Q)}{\left(\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}\right)^{2}}-\frac{(p-Q)^{2}+\mu_{\mathrm{UV}}^{2}}{\left(\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}\right)^{2}}+\frac{[2 \bar{k} \cdot(p-Q)]^{2}}{\left(\bar{k}^{2}-\mu_{\mathrm{UV}}^{2}\right)^{3}}+\mathcal{O}\left(\frac{1}{|\bar{k}|^{5}}\right)
$$

We can always add finite terms to the subtraction terms. For the ultraviolet subtraction terms we choose the finite terms such that the finite parts of the integrated ultraviolet subtraction terms are independent of $Q$ and proportional to the pole part, with the same constant of proportionality for all ultraviolet subtraction terms. This ensures that the sum of all integrated UV subtraction terms is again proportional to a tree-level amplitude [167].

### 3.4 CONTOUR DEFORMATION

Having a complete list of ultraviolet and infrared subtraction terms at hand, we can ensure that the integration over the loop momentum gives a finite result and can therefore be performed in four dimensions. However, this does not yet imply that we can safely integrate each of the four components of the loop momentum $k^{\mu}$ from minus infinity to plus infinity along the real axis. There is still the possibility that some of the loop propagators go on-shell for real values of the loop momentum. If the contour is not pinched this is harmless, as we may escape into the complex plane in a direction indicated by Feynman's $+i \delta$-prescription. However, it implies that the integration should be done over a region of real dimension 4 in the complex space $\mathbb{C}^{4}$. Let us consider an integral corresponding to a primitive one-loop amplitude with $n$ propagators minus the appropriate IR- and UV-subtraction terms:

$$
\begin{equation*}
\int \frac{d^{4} \tilde{k}}{(2 \pi)^{4}}\left(\mathcal{G}_{\mathrm{bare}}^{(1)}-\mathcal{G}_{\mathrm{soft}}^{(1)}-\mathcal{G}_{\mathrm{coll}}^{(1)}-\mathcal{G}_{\mathrm{UV}}^{(1)}\right)=\int \frac{d^{4} \tilde{k}}{(2 \pi)^{4}} P(\tilde{k}) \prod_{j=1}^{n} \frac{1}{\tilde{k}_{j}^{2}-m_{j}^{2}+i \delta} \tag{28}
\end{equation*}
$$

where $P(\tilde{k})$ is a polynomial of the loop momentum $\tilde{k}^{\mu}$ and the integration is over a complex contour in order to avoid whenever possible the poles of the propagators. We set $\tilde{k}^{\mu}=k^{\mu}+i \kappa^{\mu}(k)$, where $k^{\mu}$ is real [170]. After this deformation our integral equals

$$
\begin{equation*}
\int \frac{d^{4} k}{(2 \pi)^{4}}\left|\frac{\partial \tilde{k}^{\mu}}{\partial k^{\nu}}\right| P(\tilde{k}(k)) \prod_{j=1}^{n} \frac{1}{k_{j}^{2}-m_{j}^{2}-\kappa^{2}+2 i k_{j} \cdot \kappa} \tag{29}
\end{equation*}
$$

To match Feynman's $+i \delta$-prescription we have to construct the deformation vector $\kappa$ such that

$$
\begin{equation*}
k_{j}^{2}-m_{j}^{2}=0 \quad \rightarrow \quad k_{j} \cdot \kappa \geq 0 \tag{30}
\end{equation*}
$$

We remark that the numerical stability of the Monte Carlo integration depends strongly on the definition of the deformation vector $\kappa$.

### 3.5 NLO results for $\mathbf{n}$-jets in electron-positron annihilation

We have calculated results for jet observables in electron-positron annihilation, where the jets are defined by the Durham jet algorithm [166]. The cross section for $n$ jets normalised to the LO cross section for $e^{+} e^{-} \rightarrow$ hadrons reads

$$
\begin{equation*}
\frac{\sigma_{n-j e t}(\mu)}{\sigma_{0}(\mu)}=\left(\frac{\alpha_{s}(\mu)}{2 \pi}\right)^{n-2} A_{n}(\mu)+\left(\frac{\alpha_{s}(\mu)}{2 \pi}\right)^{n-1} B_{n}(\mu)+\mathcal{O}\left(\alpha_{s}^{n}\right) . \tag{31}
\end{equation*}
$$

One can expand the perturbative coefficient $A_{n}$ and $B_{n}$ in $1 / N_{c}$ :

$$
A_{n}=N_{c}\left(\frac{N_{c}}{2}\right)^{n-2}\left[A_{n, \mathrm{lc}}+\mathcal{O}\left(\frac{1}{N_{c}}\right)\right], \quad B_{n}=N_{c}\left(\frac{N_{c}}{2}\right)^{n-1}\left[B_{n, \mathrm{lc}}+\mathcal{O}\left(\frac{1}{N_{c}}\right)\right] .
$$

We calculate the leading order coefficient $A_{n, \text { lc }}$ and the next-to-leading order coefficient $B_{n, \text { lc }}$ for $n \leq 7$ at the renormalisation scale $\mu$ equal to the centre-of-mass energy. The centre-of-mass energy is taken to be equal to the mass of the $Z$-boson. The scale variation can be restored from the renormalisation group equation. The calculation is done with five massless quark flavours. Fig. 5 ]shows the comparison of our




Fig. 5: Comparison of the NLO corrections to the two-, three- and four-jet rate between the numerical calculation and an analytic calculation. The error bars from the Monte Carlo integration are shown and are almost invisible.
numerical approach with the well-known results for two, three and four jets [179, 180, 181]. We observe an excellent agreement. The results for five, six and seven jets for the jet parameter $y_{c u t}=0.0006$ are

$$
\begin{array}{ll}
\frac{N_{c}^{4}}{8} A_{5, \mathrm{lc}}=(2.4764 \pm 0.0002) \cdot 10^{4}, & \frac{N_{c}^{5}}{16} B_{5, \mathrm{lc}}=(1.84 \pm 0.15) \cdot 10^{6}, \\
\frac{N_{c}^{5}}{16} A_{6, \mathrm{lc}}=(2.874 \pm 0.002) \cdot 10^{5}, & \frac{N_{c}^{6}}{32} B_{6, \mathrm{lc}}=(3.88 \pm 0.18) \cdot 10^{7}, \\
\frac{N_{c}^{6}}{32} A_{7, \mathrm{lc}}=(2.49 \pm 0.08) \cdot 10^{6}, & \frac{N_{c}^{7}}{64} B_{7, \mathrm{lc}}=(5.4 \pm 0.3) \cdot 10^{8} . \tag{32}
\end{array}
$$

### 3.6 FIRST STEPS TOWARDS NNLO

An NNLO calculation requires among other things also the calculation of the one-loop amplitude squared. The expansion in the dimensional regularisation parameter $\varepsilon$ of the one-loop amplitude starts at order $(-2)$ one would naively expect that up to order $\varepsilon^{0}$ the $\mathcal{O}(\uparrow)$ - and $\mathcal{O}\left(\varepsilon^{2}\right)$-terms of the one-loop amplitude are needed for an NNLO calculation. However, it is by no means obvious how the approaches for one-loop amplitudes based on unitarity or the numerical method can be extended to include the higherorder terms in the $\varepsilon$-expansion. It turns out that the computation of these higher-order terms can be avoided, provided a method is known to compute the finite two-loop remainder function. The one- and two-loop amplitudes can be written as [182]

$$
\begin{align*}
\mathcal{A}^{(1)} & =\mathbf{Z}^{(1)} \mathcal{A}^{(0)}+\mathcal{F}_{\text {minimal }}^{(1)}, \\
\mathcal{A}^{(2)} & =\left(\mathbf{Z}^{(2)}-\mathbf{Z}^{(1)} \mathbf{Z}^{(1)}\right) \mathcal{A}^{(0)}+\mathbf{Z}^{(1)} \mathcal{A}^{(1)}+\mathcal{F}_{\text {minimal }}^{(2)}, \tag{33}
\end{align*}
$$

where the operators $\mathbf{Z}^{(1)}$ and $\mathbf{Z}^{(2)}$ contain all the infrared poles and $\mathcal{F}_{\text {minimal }}^{(1)}$ and $\mathcal{F}_{\text {minimal }}^{(2)}$ are finite remainders. Here we used the convention that the operators $\mathbf{Z}^{(1)}$ and $\mathbf{Z}^{(2)}$ contain only pole terms, but no terms of order $\varepsilon^{k}$ with $k \geq 0$. This corresponds to a minimal scheme. The operators $\mathbf{Z}^{(1)}$ and $\mathbf{Z}^{(2)}$ are well-known. At NNLO it is sufficient to know the $\varepsilon^{0}$-terms of $\mathcal{F}_{\text {minimal }}^{(1)}$ and $\mathcal{F}_{\text {minimal }}^{(2)}$, the $\varepsilon^{1}$ - or $\varepsilon^{2}$-terms of $\mathcal{A}^{(1)}$ or $\mathcal{F}_{\text {minimal }}^{(1)}$ are not required [183].

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## 4. TOWARDS THE AUTOMATION OF ONE-LOOP AMPLITUDES ${ }^{6}$


#### Abstract

A program is presented that computes one-loop amplitudes automatically for processes with up to 6 external particles based on the Feynman-diagram approach. Additionally, universal one-loop building blocks, which can be used to compute several processes at NLO QCD are calculated.


### 4.1 INTRODUCTION

The calculation of processes with multi-particle final states beyond the leading order approximation has been an active field of research during the last years as a consequence of the demand of high accuracy for signal and background processes at the LHC. A next-to-leading (NLO) calculation consists of virtual and real radiation processes which are infrared divergent (IR) separately and can be computed numerically only after extracting the divergences of the real radiation contributions. The one-loop virtual calculation for multiple particles poseses a challenge of complexity not only due to the large number of contributing diagrams, but also concerning the stability of the numerical code to evaluate them. In the last years, an enormous progress has been achieved applying new techniques and using traditional Feynman-diagram approach, leading to new NLO predictions.

Due to the large number of processes of potential interest at the LHC, the scientific community has worked in the automation of the NLO calculations. The automation of the real contributions including their infrared subtraction terms has been successfully implemented in several packages and the automation of the virtual corrections, which is a harder problem, is currently being achieved in several programs (see [184] and references therein).

In Ref. [185], the early stage of a program, in the framework of Mathematica [186] and FeynCalc [187], to compute automatically one-loop amplitudes based on traditional Feynman-diagram techniques and involving up to $2 \rightarrow 4$ processes was presented. This program will become publicly available in the future. The method used is described in Section 4.2. In Section 4.3, we present a set of universal one-loop building blocks that has been used to compute recently several processes included in the VBFNLO package [42, 41].

### 4.2 TOWARDS AN AUTOMATIC ONE-LOOP AMPLITUDE GENERATOR

The program above mentioned automatically simplifies a set of amplitudes up to Hexagons of rank 5. The result is given in terms of scalar and tensor integrals following the Passarino-Veltman convention [112, 185], spinor chains, polarization vectors and model parameters. The simplified expression is written automatically to FORTRAN routines. For massless propagators, the amplitudes can be evaluated also in Mathematica with unlimited precision, which is used for testing purposes. To achieve that, the scalar integrals, the tensor reduction formalism to extract the tensor coefficient integrals, and also the helicity method described in Ref. [188, 189] to compute the spinor products have been implemented at

[^196]the FORTRAN and Mathematica level. For the determination of the tensor integrals up to the box level, the Passarino-Veltman tensor reduction formalism [112] is used applying the LU decomposition method to avoid the explicit calculation of inverse Gram matrices by solving a system of linear equations, which is a more stable procedure close to singular points. Finally, for singular Gram determinants, special tensor reduction routines following Ref. [115] have been implemented, however, the external momenta convention (Passarino-like) was used. The impact of these methods is discussed in detail in Ref. [185]. For pentagons, in addition to the Passarino-Veltman formalism, the method proposed by Denner and Dittmaier [115, 190], applied also to hexagons, has been implemented. For that, the recursion relations of Ref. [115] in terms of the Passarino-Veltman external momenta convention have been re-derived. This last method is used for the numerical implementation at the FORTRAN level.

The Mathematica function does several algebraic manipulations that are summarized as follows:

- Simultaneous extraction of rational terms based on Dirac algebra manipulations and cancelation of scalar products against propagators.
- Reduction to a minimal basis of tensor and scalar integrals.
- Reduction to a minimal basis of spinor chains.
- The use of Chisholm identities, which are only valid in 4 dimensions, for the contraction of Lorentz indices among different spinor chains is applied, if selected.
- Factorization of loop dependent and independent factors (Useful to perform gauge tests, Ward identities or the re-evaluation of the amplitudes for different helicity polarization of gluons and fermions at a lower CPU cost).
As an example of the notation used, the following Hexagon diagram is used. This is written as follows:

where $g_{0}$ is the strong unrenormalized coupling, $\mathcal{C}_{i j}^{V_{1} V_{2} V_{3} V_{4}}$ is a color diagram dependent factor, e.g, $\mathcal{C}_{i j}^{\gamma \gamma g \gamma}=\left(T_{a}\right)_{i j}\left(C_{F}-1 / 2 C_{A}\right) . g_{\tau}^{V_{i} f}$ are electroweak couplings and $\mathcal{M}_{\tau}^{i j}$ represents the amplitude considering generic off-shell vector bosons with color indices $i j$ for a given helicity $\tau$. The amplitude $\mathcal{M}_{\tau}^{i j}$, omitting color indices, is written in terms of

$$
\begin{equation*}
\mathcal{M}_{\tau}=\mathcal{M}_{\tau}^{D=4}+(D-4) \mathcal{M}_{\tau}^{D R} \tag{35}
\end{equation*}
$$

where $\mathcal{M}_{\tau}^{D=4}$ is the amplitude that one would obtain performing the Dirac algebra manipulation in four dimensions, $D=4$, and $\mathcal{M}_{\tau}^{D R}$ contains the rational terms and vanishes in Dimensional Reduction $(D R)$. These functions are decomposed in the form:

$$
\begin{equation*}
\mathcal{M}^{(D=4, D R)}=\sum_{i, j} \mathrm{SM}_{i, \tau} \mathrm{Fl}_{j}, \tag{36}
\end{equation*}
$$

where $\mathrm{SM}_{i, \tau}$ is a basis of Standard Matrix elements corresponding to spinor products describing the quark line of Eq. (34] which are computed following the helicity method [188, 189] with a defined helicity, $\tau . \mathrm{F1}_{j}$ are complex functions which are further decomposed into dependent and independent loop integral parts,

$$
\begin{equation*}
\mathrm{F}_{j}=\sum_{l, k} \mathrm{~F}_{l} T_{k}\left(\epsilon\left(p_{n}\right) \cdot p_{m} ; \epsilon\left(p_{i}\right) \cdot \epsilon\left(p_{r}\right)\right) \tag{37}
\end{equation*}
$$

$T_{k}$ is a monomial function at most for each polarization vector $\epsilon\left(p_{x}\right)$, i.e., $\epsilon\left(p_{x}\right)^{0}$ or $\epsilon\left(p_{x}\right)^{1}$. The first possibility, $\epsilon\left(p_{x}\right)^{0}$, implies that the polarization vector appears in the set of Standard Matrix elements
$\mathrm{SM}_{i, \tau} . F_{l}$ contains kinematic variables $\left(p_{i} \cdot p_{j}\right)$, the scalar integrals ( $B_{0}, C_{0}, D_{0}$ ), and the tensor integral coefficients $\left(B_{i j}, C_{i j}, D_{i j}, E_{i j}, F_{i j}\right)$. Then, the full result is obtained from $\mathcal{M}_{\tau}^{D=4}$ and $\mathcal{M}_{\tau}^{D R}$ using the finite and the coefficients of the $1 / \epsilon^{n}$ poles of the scalar and tensor coefficient integrals:

$$
\begin{equation*}
\mathcal{M}_{v}^{D=4}=\widetilde{\mathcal{M}}_{v}+\frac{\mathcal{M}_{v}^{1}}{\epsilon}+\frac{\mathcal{M}_{v}^{2}}{\epsilon^{2}}, \quad(D-4) \mathcal{M}_{v}^{D R}=\widetilde{\mathcal{N}}_{v}+\frac{\mathcal{N}_{v}^{1}}{\epsilon} \tag{38}
\end{equation*}
$$

where, e.g., $\widetilde{\mathcal{M}}_{v}$ is the finite contribution obtained using the finite pieces of the scalar and tensor coefficient integrals including the finite contributions from rational terms arising in ultraviolet tensor coefficient integrals.

### 4.3 UNIVERSAL BUILDING BLOCKS

Based on the observation that the same one-loop virtual amplitudes appear in many processes (Fig. 6), we are aiming to collect a basis of universal building blocks, which can be used to compute all of the $2 \rightarrow 4$ processes at LHC at the QCD one-loop level (Similar to the philosophy of older versions of MADGRAPH [191] calling the HELAS [192] routines). This methodology of collecting topologies in groups has been proved very successful in the program VBFNLO, where for example a boxline routine, first line of Fig. 6, is computed and applied to $p p \rightarrow V V, p p \rightarrow V V V, p p \rightarrow V V j$ and EW production of $p p \rightarrow V j j$ and $p p \rightarrow H V j j$.


Fig. 6: Boxline contributions appearing in different processes.

To do that, we use the effective current approach described and applied in Refs. [39, 47, 31, 193, 21]. As illustration, the first diagram of the second raw of Fig. 6is used. This can be written as,

$$
\begin{equation*}
A_{V_{1} V_{2} V_{3} V_{4}, \tau}=J_{V_{1}^{*}}^{\mu_{1}} J_{V_{2}^{*}}^{\mu_{2}} \mathcal{M}_{\mu_{1} \mu_{2}, \tau} \equiv \mathcal{M}_{V_{1}^{*} V_{2}^{*}, \tau} \tag{39}
\end{equation*}
$$

where the color indices have been omitted. Here, $J_{V_{1}^{*}}^{\mu_{1}}$ and $J_{V_{2}^{*}}^{\mu_{2}}$ represent effective polarization vectors in the unitarity gauge for the EW sector including finite width effects in the scheme of Refs. [194, 195] and propagator factors, e.g.,

$$
\begin{equation*}
J_{V_{1}^{*}}^{\mu_{1}}\left(q_{1}\right)=\frac{-i}{q_{1}^{2}-M_{V_{1}^{*}}^{2}-i M_{V_{1}^{*}} \Gamma_{V_{1}^{*}}}\left(g_{\mu}^{\mu_{1}}-\frac{q_{1}^{\mu_{1}} q_{1 \mu}}{q_{1}^{2}-M_{V_{1}^{*}}^{2}-i M_{V_{1}^{*}} \Gamma_{V_{1}^{*}}}\right) \Gamma_{V_{1}^{*} V_{1} V_{3}}^{\mu} \tag{40}
\end{equation*}
$$

with $\Gamma_{V_{1}^{*}}$, the width of the $V_{1}^{*}$ vector boson, and $\Gamma_{V_{1}^{*} V_{1} V_{3}}^{\mu}$, the triple vertex, which can also contain the leptonic decay of the EW vector bosons including all off-shell effects or BSM physics. In this manner, we can then concentrate in computing, instead of $A_{V_{1} V_{2} V_{3} V_{4}, \tau}$, the virtual correction to two massive vector bosons attached to the quark line, $\mathcal{M}_{V_{1}^{*} V_{2}^{*}, \tau}$, or equivalently $\mathcal{M}_{\mu_{1} \mu_{2}, \tau}$, where the polarization vectors or effective currents have been factored out. In our approach, this basic building block is the so-called Boxline, which is computed only once and re-used in different processes.

We plan to do a classification of all the topologies that appear at 1 loop level for up to $2 \rightarrow 4$ processes and install a library with all the basic one-loop building blocks already computed and simplified. This would be an advantage since, for example for $q q \rightarrow V V V V$ production, up to 24 hexagons for a single subprocess would appear, corresponding to the permutations of the vector bosons on the hexagon of Eq. 34. In this approach, the amplitude is obtained by calling the same one-loop amplitude 24 times with the corresponding ordering of momenta and polarization vectors. We aim towards an automation of this procedure, which will result into a faster and shorter final FORTRAN code generation. The specific building blocks are collected into groups with specific gauge and IR factorization properties, e.g, factorization of the IR divergences against the corresponding born, known behavior under Ward identity checks.

In Fig. 7. we present the topologies that have been computed and tested. In the first line, corrections to a quark line with the emission of $\mathrm{V}_{n}$ vector bosons in a fixed order are represented for 4 different topologies. (The first 2 were explained in detail in Ref. [185], including their stability behavior). We have only depicted the virtual amplitude with the higher complexity for a giving building block, e.g. the boxline of Fig.6is obtained from the first diagram with two vector bosons attached, i.e., $n=2$ in $V_{n}$. The first two topologies of the second line are collected by putting together all possible Feynman-diagrams with a fixed order of the vector bosons and attaching it to the quark lines in all possible ways. The crossing of the fermion lines are treated as independent building blocks and are not depicted. Finally, the fermion-loop corrections for a fixed order of vector bosons, $V_{n}$, are computed in the last diagram of the second line

The use of modular structure routines, as the above presented, has been proved to be an advantage in the program VBFNLO [42, 41] since once a structure is computed and checked it can be re-used for different processes. For example, using the building blocks of the first and second topology together with the fermion-loop diagrams, results at NLO QCD for all $V V V$ [39, 47, 46, 45, 43, 44], several $V V j$ [31, 32, 196, 197], $H \gamma j j$ [198] and $W \gamma \gamma j$ [21] production channels have been computed recently. The last one representing the first calculation at this accuracy falling in the category of $V V V+j$ production. Up to the pentagon level, these building blocks are publicly available as part of the VBFNLO [42, 41] package together with the tensor reduction routines, excluding the routines for small Gram determinants which will become available in the future, in addition to the other building blocks.

### 4.4 CONCLUSIONS

A program which automatically evaluates one-loop amplitudes for up to $2 \rightarrow 4$ processes has been presented based on the traditional Feynman-diagram approach. The program has been developed in the framework of Mathematica and FeynCalc and writes down automatically the simplified expression to FORTRAN. Up to the pentagon level and for massless propagators, the code can be evaluated numerically inside Mathematica with unlimited precision which can be used for testing purposes. For the reduction of tensor integrals, we have developed a library that includes expansion for small Gram determinants. Using the leptonic tensor formalism, we are building a library of universal one-loop building blocks, which can be used to compute several processes at NLO QCD. Recently, following this strategy, we have reported results for all $V V V$ [39, 47, 46, 45, 43, 44], several $V V j$ [31, 32, 196, 197], $H \gamma j j$ [198] and $W \gamma \gamma j$ [21] production channels inside the VBFNLO collaboration. The ultimate goal is to generalize the library to compute all of the $2 \rightarrow 4$ processes at LHC at the QCD one-loop level, similar to the philosophy of older versions of MADGRAPH [191] calling the HELAS [192] routines,


Fig. 7: Topologies of universal building one-loop blocks. Only the most complicated diagram of each topology is depicted, e.g, the boxline of Fig 6 is obtained from the first diagram with two vector bosons attached, i.e., $V_{n}, n=2$.
and deliver a Mathematica package compatible with FeynArts [132], which can be used to compute full one-loop amplitudes automatically using the universal building blocks, resulting into a faster and shorter code generation.

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## 5. THE TWO-LOOP QCD VIRTUAL AMPLITUDE FOR W PAIR PRODUCTION WITH FULL MASS DEPENDENCE 7

### 5.1 INTRODUCTION

One of the main aims in the Large Hadron Collider (LHC) physics program is undoubtedly the discovery (or the exclusion) of the Higgs boson which is responsible for the fermion and gauge boson masses and also part of the mechanism of dynamical breaking of the Electroweak (EW) symmetry. Another important goal for the LHC is the precise measurement of the hadronic production of gauge boson pairs, $W W, W Z, Z Z, W \gamma, Z \gamma$, this in connection to the investigation of the non-Abelian gauge structure of the SM . W pair production,

$$
\begin{equation*}
q \bar{q} \rightarrow W^{+} W^{-}, \tag{41}
\end{equation*}
$$

[^197]plays an essential role as it serves as a signal process in the search for New Physics and also is the dominant irreducible background to the Higgs discovery channel $p p \rightarrow H \rightarrow W^{*} W^{*} \rightarrow l \bar{\nu} \bar{l}^{\prime} \nu^{\prime}$, in the intermediate Higgs mass range [199]. Both ATLAS and CMS collaborations have released first values for the $W W$ cross section [200, 201].

The process (41) is currently known at next-to-leading order (NLO) accuracy [202, 203, 204, 205, 206, 157, ?]. The NLO corrections were proven to be large enhancing the tree-level result by almost $70 \%$ which falls to a (still) large $30 \%$ after imposing a jet veto. Therefore, if a theoretical estimate for the W pair production is to be compared against experimental measurements at the LHC, one is bound to go one order higher in the perturbative expansion, namely, to the next-to-next-to-leading order (NNLO). This would allow, in principle, an accuracy of around $10 \%$.

High accuracy for the W pair production is also needed when the process is studied as background to Higgs production in order to match accuracies between signal and background. The signal process for the Higgs discovery via gluon fusion, $g g \rightarrow H$, as well as the process $H \rightarrow W W \rightarrow l \bar{\nu} \bar{l}^{\prime} \nu^{\prime}$ are known at NNLO [207, 208, 209, 210, 211, 212, 213, 214, 215, 216], whereas the EW corrections are known beyond NLO [217]. Another process that needs to be included in the background is the W pair production in the loop induced gluon fusion channel,

$$
\begin{equation*}
g g \rightarrow W^{+} W^{-} \tag{42}
\end{equation*}
$$

The latter contributes at $\mathcal{O}\left(\alpha_{s}^{2}\right)$ relative to the quark-anti-quark-annihilation channel but is nevertheless enhanced due to the large gluon flux at the LHC [218, 219].

The first main difficulty in studying the NNLO QCD corrections for W pair production is the calculation of the two-loop virtual amplitude since it is a $2 \rightarrow 2$ process with massive external particles. We have already computed the virtual corrections at the high energy limit [220, 97, 221]. However, this is not enough as it cannot cover the kinematical region close to threshold. Therefore, in order to cover all kinematical regions we proceed as follows. We perform a deep expansion in the W mass around the high energy limit which in combination with the method of numerical integration of differential equations [222, 223, 224] allows us the numerical computation of the two-loop amplitude with full mass dependence over the whole phase space.

### 5.2 THE HIGH ENERGY LIMIT

The methodology for obtaining the massive amplitude in the high energy limit, namely the limit where all the invariants are much larger than the W mass, is similar to the one followed in Refs. [225, 226]. The amplitude is reduced to an expression that only contains a small number of integrals (master integrals) with the help of the Laporta algorithm [227]. In the calculation for the two-loop amplitude there are 71 master integrals. Next step is the construction, in a fully automatised way, of the Mellin-Barnes (MB) representations [228, 229] of all the master integrals by using the MBrepresentation package [230]. The representations are then analytically continued in the number of space-time dimensions by means of the MB package [231], thus revealing the full singularity structure. An asymptotic expansion in the mass parameter ( W mass) is performed by closing contours and the integrals are finally resummed, either with the help of XSummer [232] or the PSLQ algorithm [233]. The result is expressed in terms of harmonic polylogarithms.

### 5.3 POWER CORRECTIONS AND NUMERICAL EVALUATION

The high energy limit by itself is not enough, as was mentioned before. The next step, following the methods applied in Ref. [234], is to compute power corrections in the W mass. Power corrections are good enough to cover most of the phase space, apart from the region near threshold as well as the regions corresponding to small angle scattering.

We recapitulate here some of the notation of Ref. [221] for completeness. The charged vectorboson production in the leading partonic scattering process corresponds to

$$
\begin{equation*}
q\left(p_{1}\right)+\bar{q}\left(p_{2}\right) \rightarrow W^{-}\left(p_{3}, m\right)+W^{+}\left(p_{4}, m\right) \tag{43}
\end{equation*}
$$

where $p_{i}$ denote the quark and W momenta and $m$ is the mass of the W boson.
We have chosen to express the amplitude in terms of the kinematic variables $x$ and $m_{s}$ which are defined to be

$$
\begin{equation*}
x=-\frac{t}{s}, \quad m_{s}=\frac{m^{2}}{s} \tag{44}
\end{equation*}
$$

where

$$
\begin{equation*}
s=\left(p_{1}+p_{2}\right)^{2} \text { and } t=\left(p_{1}-p_{3}\right)^{2}-m^{2} \tag{45}
\end{equation*}
$$

The variation then of $x$ within the range $[1 / 2(1-\beta), 1 / 2(1+\beta)]$, where $\beta=\sqrt{1-4 m^{2} / s}$ is the velocity, corresponds to angular variation between the forward and backward scattering.

It should be evident that any master integral $M_{i}$ can be written then as

$$
\begin{equation*}
M_{i}=M_{i}\left(m_{s}, x, \epsilon\right)=\sum_{j=k}^{l} \epsilon^{j} I_{i j}\left(m_{s}, x\right) \tag{46}
\end{equation*}
$$

where $\epsilon$ is the usual regulator in dimensional regularization $(d=4-2 \epsilon)$ and the lowest power of $\epsilon$ in the sum can be -4 .

The crucial point now is that the derivative of any Feynman integral with respect to any kinematical variable is again a Feynman integral with possibly higher powers of denominators or numerators which can also be reduced anew in terms of the initial set of master integrals. This means that one can construct a partially triangular system of differential equations in the mass, which can subsequently be solved in the form of a power series expansion, with the expansion parameter in our case being $m_{s}$ following the conventions above.

Let us differentiate with respect to $m_{s}$ and $x$, we will then have respectively

$$
\begin{equation*}
m_{s} \frac{d}{d m_{s}} M_{i}\left(m_{s}, x, \epsilon\right)=\sum_{j} C_{i j}\left(m_{s}, x, \epsilon\right) M_{j}\left(m_{s}, x, \epsilon\right) \tag{47}
\end{equation*}
$$

and

$$
\begin{equation*}
x \frac{d}{d x} M_{i}\left(m_{s}, x, \epsilon\right)=\sum_{j} C_{i j}^{\prime}\left(m_{s}, x, \epsilon\right) M_{j}\left(m_{s}, x, \epsilon\right) \tag{48}
\end{equation*}
$$

We use Eq. 47) to obtain the mass corrections for the master integrals calculating the power series expansion up to order $m_{s}^{11}$ (see also Ref. [234] for more details). This deep expansion in $m_{s}$ should be sufficient for most of the phase space but still not enough to cover the whole allowed kinematical region. The way to proceed from this point is to numerically integrate the system of differential equations.

In particular, we choose to work with the master integrals in the form of Eq. 46, where the $\epsilon$ dependence is explicit. We can then work with the coefficients of the $\epsilon$ terms and accordingly have

$$
\begin{equation*}
m_{s} \frac{d}{d m_{s}} I_{i}\left(m_{s}, x\right)=\sum_{j} J_{i j}^{M}\left(m_{s}, x\right) I_{j}\left(m_{s}, x\right) \tag{49}
\end{equation*}
$$

and

$$
\begin{equation*}
x \frac{d}{d x} I_{i}\left(m_{s}, x\right)=\sum_{j} J_{i j}^{X}\left(m_{s}, x\right) I_{j}\left(m_{s}, x\right) \tag{50}
\end{equation*}
$$

where the Jacobian matrices $J^{M}$ and $J^{X}$ have rational function elements.

By using this last system of differential equations, one can obtain a full numerical solution to the problem. What we are essentially dealing now with is an initial value problem and the main requirement is to have the initial conditions to proper accuracy. The initial conditions, namely the values of the master integrals at a proper kinematical point which we call initial point, are provided by the power series expansion. The initial point has to be chosen somewhere in the high energy limit region, where $m_{s}$ is small and therefore, the values obtained by the power series are very accurate. Starting from there, one can evolve to any other point of the phase space by numerically integrating the system of differential equations Eq. (49) and Eq. (50).

We parametrise with a suitable grid of points the region close to threshold and then we calculate the master integrals for all points of the grid by evolving as described previously. Given that the master integrals have to be very smooth (we remain above all thresholds) one can use, after having the values for the grid points, interpolation to get the values at any point of the region. We use 1600 points for the grid and take as initial conditions the values of the master integrals at the point $m_{s}=5 \times 10^{-3}, x=1 / 4$. The relative errors at that point were estimated not to exceed $10^{-18}$.

The numerical integration is performed by using one of the most advanced software packages implementing the variable coefficient multistep method (ODEPACK) [235]. We use quadruple precision to maximise accuracy. The values at any single grid point can be obtained in about 15 minutes in average (with a typical 2 GHz Intel Core 2 Duo system) after compilation with the Intel Fortran compiler. The accuracy is around 10 digits for most of the points of the grid. It is also worth noting that in order to perform the numerical integration one needs to deform the contour in the complex plane away from the real axis. This is due to the fact that along the real axis there are spurious singularities. We use an elliptic contour and we achieve a better estimate of the final global error by calculating more than once for each point of the grid, using each time different eccentricities. Grids of solutions can actually be constructed, which will be subsequently interpolated when implemented as part of a Monte Carlo program.

One very stringent test we use to cross-check the correctness and also the accuracy of our calculation is to compare the infrared pole structure of our two-loop result against the one predicted by Catani [182] (see also Refs. [236, 237, 238]). According to Catani, the infrared poles of the interference of the tree and the two-loop amplitudes follow a generic formula which in our case, since we work with the rescaled variables $m_{s}$ and $x$, can be cast into the following form:

$$
\begin{equation*}
\mathcal{C}_{\text {atani }}^{(0 \times 2)}\left(m_{s}, x, \frac{s}{\mu}\right)=2 \operatorname{Re}\left\{\mathrm{I}^{(1)}(\mathrm{ffl})\left\langle\mathrm{M}^{(0)} \mid \mathrm{M}^{(1)}\right\rangle+\mathrm{I}^{(2)}(\mathrm{ff})\left\langle\mathrm{M}^{(0)} \mid \mathrm{M}^{(0)}\right\rangle\right\} \tag{51}
\end{equation*}
$$

where $\mathrm{M}^{(0)}$ and $\mathrm{M}^{(1)}$ are the tree level and one-loop amplitudes respectively and $\mu$ is the renormalization scale. The operators $\mathrm{I}^{(1)}(\mathrm{ffl})$ and $\mathrm{I}^{(2)}(\mathrm{ffl})$ encode the information for the infrared pole structure and their exact expressions can be found in Ref. [97].

The way to perform the test is straightforward. For each point of the grid with coordinates $\left(m_{s(i)}, x_{(i)}\right)$, we compute the numerical value of the two-loop amplitude $\left(\mathrm{M}^{(2)}\right)$ interfered with the tree level amplitude

$$
\begin{equation*}
\mathcal{A}^{(0 \times 2)}\left(m_{s(i)}, x_{i}, \frac{s}{\mu}\right)=\left\langle\mathrm{M}^{(0)} \mid \mathrm{M}^{(2)}\right\rangle+\left\langle\mathrm{M}^{(2)} \mid \mathrm{M}^{(0)}\right\rangle \tag{52}
\end{equation*}
$$

by numerically integrating the differential equations as described previously and we also calculate the numerical value of the quantity $\mathcal{C}_{\text {atani }}^{(0 \times 2)}\left(m_{s(i)}, x_{(i)}, \frac{s}{\mu}\right)$ by using Eq. 51). Then, all we need to make sure is that the infrared singularities of the quantity $\left\{\mathcal{A}^{(0 \times 2)}\left(m_{s(i)}, x_{i}, \frac{s}{\mu}\right)-\mathcal{C}_{\text {atani }}^{(0 \times 2)}\left(m_{s(i)}, x_{i}, \frac{s}{\mu}\right)\right\}$ cancel numerically for every point $\left(m_{s(i)}, x_{(i)}\right)$ of the grid (ultraviolet divergencies have been removed by renormalization). We will not present here any numbers since the aim was to describe the general methods. The details and the results of the study will be presented in a future publication [239].

### 5.4 CONCLUSIONS

W pair production via quark-anti-quark-annihilation is an important signal process in the search for New Physics as well as the dominant irreducible background for one of the main Higgs discovery channels: $H \rightarrow W W \rightarrow 4$ leptons. Therefore, the accurate knowledge of this process is essential for the LHC. After having calculated the two-loop and the one-loop-squared virtual QCD corrections to the W boson pair production in the high energy limit we proceed to the next step. Namely, we use a combination of a deep expansion in the W mass around the high energy limit and of numerical integration of differential equations to compute the two-loop amplitude with full mass dependence over the whole phase space. A strigent cross-check of our calculation is to verify that the infrared structure of our result agrees with the prediction of the Catani formalism for the infrared structure of QCD amplitudes.

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## 6. COMPUTATION OF INTEGRATED SUBTRACTION TERMS NUMERICALLY ${ }^{8}$


#### Abstract

We report on a numerical representation of the integrated subtraction terms of the NNLO subtraction scheme defined in Refs. [240, 241, 242, 243]. The integrated approximate cross sections themselves can be written as products of insertion operators (in colour space) times the Born, or the one-loop cross section. The insertion operator is constructed from the numerical representation of the integrated subtraction terms. We give selected results for the integrated doubly-collinear subtraction term.


### 6.1 INTRODUCTION

We consider the NNLO correction to a generic $m$-jet observable,

$$
\begin{equation*}
\sigma^{\mathrm{NNLO}}=\int_{m+2} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}} J_{m+2}+\int_{m+1} \mathrm{~d} \sigma_{m+1}^{\mathrm{RV}} J_{m+1}+\int_{m} \mathrm{~d} \sigma_{m}^{\mathrm{VV}} J_{m} . \tag{53}
\end{equation*}
$$

The three contributions on the right hand side are separately divergent in $d=4$ dimensions, but their sum is finite for IR safe observables. To obtain the finite NNLO correction, we first continue analytically all integrals to $d=4-2 \epsilon$ dimensions and then rewrite Eqn. (53) as

$$
\begin{equation*}
\sigma^{\mathrm{NNLO}}=\int_{m+2} \mathrm{~d} \sigma_{m+2}^{\mathrm{NNLO}}+\int_{m+1} \mathrm{~d} \sigma_{m+1}^{\mathrm{NNLO}}+\int_{m} \mathrm{~d} \sigma_{m}^{\mathrm{NNLO}} \tag{54}
\end{equation*}
$$

that is a sum of three integrals where the integrands,

$$
\begin{gather*}
\mathrm{d} \sigma_{m+2}^{\mathrm{NNLO}}=\left\{\mathrm{d} \sigma_{m+2}^{\mathrm{RR}} J_{m+2}-\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{2}} J_{m}-\left[\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}} J_{m+1}-\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{12}} J_{m}\right]\right\}_{\epsilon=0},  \tag{55}\\
\mathrm{~d} \sigma_{m+1}^{\mathrm{NNLO}}=\left\{\left[\mathrm{d} \sigma_{m+1}^{\mathrm{RV}}+\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}}\right] J_{m+1}-\left[\mathrm{d} \sigma_{m+1}^{\mathrm{RV}, \mathrm{~A}_{1}}+\left(\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}}\right)^{\mathrm{A}_{1}}\right] J_{m}\right\}_{\epsilon=0}, \tag{56}
\end{gather*}
$$

and

$$
\begin{equation*}
\mathrm{d} \sigma_{m}^{\mathrm{NNLO}}=\left\{\mathrm{d} \sigma_{m}^{\mathrm{VV}}+\int_{2}\left[\mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{2}}-\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{12}}\right]+\int_{1}\left[\mathrm{~d} \sigma_{m+1}^{\mathrm{RV}, \mathrm{~A}_{1}}+\left(\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{~A}_{1}}\right)^{\mathrm{A}_{1}}\right]\right\}_{\epsilon=0} J_{m}, \tag{57}
\end{equation*}
$$

[^198]are integrable in four dimensions by construction. The approximate cross sections $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{2}}$ and $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}$ regularise the doubly- and singly-unresolved limits of the real-emission contribution, $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}}$ respectively. The double subtraction due to the overlap of these two terms is compensated by $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{12}}$. These terms are given explicitly in Ref. [242]. Finally, $\mathrm{d} \sigma_{m+1}^{\mathrm{RV}, \mathrm{A}_{1}}$ and $\left(\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}\right)^{\mathrm{A}_{1}}$ regularise the singly-unresolved limits of $\mathrm{d} \sigma_{m+1}^{\mathrm{RV}}$ and $\int_{1} \mathrm{~d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}$ respectively. They are given explicitly in Ref. [243].

The construction of each approximate cross section in Eqns. (55-57) is based on the known and universal IR limits of tree level and one-loop squared matrix elements, and proceeds in two steps. First, the IR factorisation formulae are written in such a way that their complicated overlap structure can be disentangled ("matching of limits") [240, 244]. Second, we define "extensions" of the formulae, so that they are unambiguously defined away from the strict IR limits [241, 242, 243]. These extensions are defined by the use of various momentum mappings that map a set of $m+1$ or $m+2$ momenta into a set of $m$ momenta,

$$
\begin{equation*}
\{p\}_{m+1} \longrightarrow\{\tilde{p}\}_{m} \quad \text { and } \quad\{p\}_{m+2} \longrightarrow\{\tilde{p}\}_{m} \tag{58}
\end{equation*}
$$

such that (i) the delicate structure of cancellations among the matched limit formulae in various limits is respected (ii) exact momentum conservation is implemented, and (iii) the original $m+1$ or $m+2$ particle phase space factorises exactly into the product of an $m$ particle phase space and a one- or two-particle phase space measure,

$$
\begin{equation*}
\mathrm{d} \phi_{m+r}\left(\{p\}_{m+r} ; Q\right)=\mathrm{d} \phi_{m}\left(\{\tilde{p}\}_{m} ; Q\right)\left[\mathrm{d} p_{r, m}\right], \quad r=1,2 . \tag{59}
\end{equation*}
$$

To finish the definition of the scheme, one must compute once and for all the one- and two-particle integrals, denoted formally as $\int_{1}$ and $\int_{2}$, appearing in Eqns. 5657 .

In general the integrated subtraction terms are integrals of extensions over the whole phase space of combinations of the QCD splitting functions and squared soft currents. In this proceedings we discuss two examples: (i) the singly-collinear subtractions $\mathcal{C}_{i r}^{(\ell, 0)}$ and (ii) the doubly-collinear subtractions $\mathcal{C}_{i r, j s}^{(0,0)}$, which are part of $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{1}}$ and $\mathrm{d} \sigma_{m+2}^{\mathrm{RR}, \mathrm{A}_{2}}$ in Eqn. 55 , respectively. The precise definitions of these terms can be found in Ref. [242]. The meaning of the superscript is irrelevant for our present purpose (also explained in Ref. [242]).

Denoting a generic subtraction term by $\mathcal{X}^{(\ell, k)}$ (such as $\mathcal{C}_{i r}^{(\ell, 0)}$ ) the integrated counterterms can be written in the following general form:

$$
\begin{equation*}
\int_{r} \mathcal{X}^{(\ell, k)}=\left[\frac{\alpha_{\mathrm{s}}}{2 \pi} S_{\epsilon}\left(\frac{\mu^{2}}{Q^{2}}\right)^{\epsilon}\right]^{r+\ell} N_{X}(\epsilon) X^{(\ell)}(x, \ldots) \operatorname{Re}\left\langle\mathcal{M}_{m}^{(0)}(\{\tilde{p}\})\right| \boldsymbol{T}_{i} \cdot \boldsymbol{T}_{j} \ldots\left|\mathcal{M}_{m}^{(k)}(\{\tilde{p}\})\right\rangle, \tag{60}
\end{equation*}
$$

where $S_{\epsilon}=(4 \pi)^{\epsilon} / \Gamma(1-\epsilon)$, and $X^{(\ell)}(x, \ldots)$ represents a function that depends on kinematical invariants of the factorized $m$-parton phase space. It results in the integration of the subtraction term $\mathcal{X}^{(\ell, k)}$ over the factorized phase spaces [ $\mathrm{d} p_{r, m}$ ] in Eqn. 59). In a NNLO computation the possible cases are $r+\ell+k=1$ with $\ell+k=0$ or 1 , and $r=2$ with $\ell+k=0$. We use the colour- and spin-state notation of Ref. [236], when the amplitude for a scattering process involving $m$ final-state momenta, $\left|\mathcal{M}_{m}^{(k)}\right\rangle$, is an abstract vector in colour and spin space; $k$ denotes the number of loops. Colour interactions at QCD vertices are represented by associating colour charges $\boldsymbol{T}_{i}$ with the emission of a gluon from each parton $i$. There are $2 r$ such colour charges. Then the functions $X^{(\ell)}$ are dimensionless in colour-space. For certain subtraction terms, universal, possibly $\epsilon$-dependent numerical factors, $N_{X}(\epsilon)$ appear naturally, which can be factored out. Our purpose is to compute all functions $X^{(\ell)}$, which we discuss next.

### 6.2 INTEGRATING THE COUNTERTERMS

The actual computation of the integrated counterterms leads to a large number of multi-dimensional integrals. The ultimate goal is to find the analytical form of the coefficients of a Laurent expansion (in
$\epsilon$ ) of these integrals, which turns out to be a rather tedious job. In order to compute these coefficients as efficiently as possible, we have explored several methods.

First, it is possible to extend the method of integration-by-parts identities and solving of differential equations, developed for computing multi-loop Feynman integrals [245, 246], to the relevant phase space integrations [247]. This method yields $\epsilon$-expansions with fully analytical coefficients, with the final results being expressed in terms of two-dimensional harmonic polylogarithms (after a suitable basis extension, see Ref. [247] for details). This approach was used successfully to compute a class of singlyunresolved integrals [247].

Second, the phase space integrals that arise can be computed via the method of Mellin-Barnes (MB) representations [228, 229, 248]. Here we obtain the $\epsilon$-expansion coefficients in terms of complex contour integrals over $\Gamma$-functions. Performing these integrals by the use of the residue theorem, a representation in terms of harmonic sums is obtained. In many cases, the sums can be evaluated in a closed form, yielding an analytical result. In some instances however, we find multi-dimensional MB integrals that are very difficult to compute fully analytically. Nevertheless, in these situations a direct numerical evaluation of the appropriate MB representations provides a fast and reliable way to obtain final results with small numerical uncertainties. We stress that for phenomenological applications, this is all that is required, since the numerical uncertainty of the complete computation is dominated by the phase space integrations. We have used the MB method to compute all singly-unresolved integrals [249], and all two-particle integrals appearing in $\int_{2} \mathrm{~d} \sigma_{m+2}^{R R, A_{12}}$ as well [91].

Finally, the method of iterated sector decomposition [250] can also be used to calculate the integrals we encounter [251]. Sector decomposition produces a representation of the $\epsilon$-expansion where the coefficients are given in terms of (mostly quite cumbersome) finite integrals over the unit hypercube. The analytical evaluation of these integrals is not feasible except for the simplest cases. Nevertheless, this method is simple to implement and can be automated to a large extent. In fact there are several computer programs that use various implementations of sector decomposition to provide numerical values of coefficients of the powers of $\epsilon$ in the Laurent expansion of dimensionally regulated integrals [252, 253, 254]. We found the program $\operatorname{SecDec}$ powerful and flexible to generate sufficiently precise values of our integrated subtraction terms.

Choosing the Cuhre integrator implemented in SecDec, we can easily reach $10^{-7}$ relative precision for the integration. Such precision is sufficient for our purposes: (i) to demonstrate the cancellation of the $\epsilon$ poles numerically, and (ii) to compute the finite integrals in Eqns. (56) and (57). As the numerical uncertainty of the second item is limited more by the Monte Carlo integration over the $m+1$ and $m$ particle phase spaces, for item (ii) much lower (not better than $10^{-3}$ ) precision is sufficient. This looser requirement on the precision for the $\mathrm{O}(1)$ terms and the fact that the integrated subtraction terms are smooth functions of their parameters, with logarithmic behaviour for asymptotically small values of the parameters, makes possible that we find sufficient approximations to the integrated subtraction terms.

### 6.3 APPROXIMATE INTEGRATED SUBTRACTION TERMS

The computation of the integrated subtraction terms at any given values of the kinematical parameters, as required in the Monte Carlo integration over the phase space, is not feasible. In order to demonstrate the cancellation of the $\epsilon$ poles numerically we can choose several randomly selected phase space points and evaluate the necessary integrals with high precision. The cancellation cannot depend on the particular phase space point. In the case of the finite remainders, in order to compute the phase space integrals in Eqns. 56 ) and (57), we are able to find sufficiently precise approximations to the integrated subtraction terms using a procedure that can be automated to high degree. The latter point is also important as there are several hundred integrals to compute. In the following, we outline our procedure for two cases: (i) an example with integrals depending on one kinematical parameter, $\left(\int_{1} \mathcal{X}^{(\ell, k)}=\int_{1} \mathcal{C}_{i r}^{(\ell, 0)}\right)$ and (ii) another example with integrals depending on two kinematical parameters, $\left(\int_{2} \mathcal{X}^{(\ell, k)}=\int_{2} \mathcal{C}_{i r, j s}^{(0,0)}\right)$.

In order to compute $\int_{1} \mathcal{C}_{i r}^{(\ell, 0)}$, we have to integrate the azimuthally averaged Altarelli-Parisi splitting functions $P_{f_{i} f_{r}}^{(\ell)}\left(z_{i, r}, z_{r, i} ; \epsilon\right)$ in $4-2 \epsilon$ dimensions for the splitting process $f_{i r} \rightarrow f_{i}+f_{r}$, with $z_{i}$ being the momentum fraction of parton $f_{i}$. It was discussed in Ref. [249] that the corresponding functions $C_{i r}^{(\ell)}$ can be expressed as combinations of the integrals (we changed the notation from $\mathcal{I}$ to $\mathcal{I}_{C}$ )

$$
\begin{equation*}
\mathcal{I}_{C}\left(x ; \epsilon, \alpha_{0}, d_{0}, \kappa, k, \delta, g_{I}^{( \pm)}\right)=\frac{16 \pi^{2}}{S_{\epsilon}} Q^{2 \epsilon} \int_{1}\left[\mathrm{~d} p_{1, m+1}^{(i r)}\right] \frac{z_{r}^{k+\delta \epsilon}}{s_{i r}^{1+\kappa \epsilon}} g_{I}^{( \pm)}\left(z_{r}\right) f\left(\alpha_{0}, \alpha_{i r}, d(m, \epsilon)\right) . \tag{61}
\end{equation*}
$$

In terms of explicit integration variables these collinear integrals have the general form [249]

$$
\begin{align*}
& \mathcal{I}_{C}\left(x ; \epsilon, \alpha_{0}, d_{0} ; \kappa, k, \delta, g_{I}^{( \pm)}\right)=x \int_{0}^{\alpha_{0}} \mathrm{~d} \alpha \alpha^{-1-(1+\kappa) \epsilon}(1-\alpha)^{2 d_{0}-1}[\alpha+(1-\alpha) x]^{-1-(1+\kappa) \epsilon} \\
& \quad \times \int_{0}^{1} \mathrm{~d} v[v(1-v)]^{-\epsilon}\left(\frac{\alpha+(1-\alpha) x v}{2 \alpha+(1-\alpha) x}\right)^{k+\delta \epsilon} g_{I}^{( \pm)}\left(\frac{\alpha+(1-\alpha) x v}{2 \alpha+(1-\alpha) x}\right) . \tag{62}
\end{align*}
$$

The necessary functions $g_{I}^{( \pm)}$are listed in Ref. [249], where analytic results of these integrals for $\alpha_{0}=1$ and $d_{0}=3$ are also presented.

Our present goal is to provide sufficiently precise numerical approximations to the functions $\mathcal{I}_{C}(x)$ in a simple way. The motivation is that often it is difficult to perform the analytic computation with arbitrary values of the parameters. For instance, the derivation with $\alpha_{0}=1$ is rather different from a derivation with $\alpha_{0}<1$. Also, the choice for $d_{0}$ is to some extent arbitrary, and a new choice requires a completely new analytic computation. Thus, for the sake of flexibility we propose a fully numerical approach here.

First we used the program SecDec, modified such that it can compute the value of the integral at multiple values of the parameter $x$ in a single run. For simplicity, we call the $\mathrm{O}(1)$ terms of the integral 'measurements'. Then, inspired by the analytic results in Ref. [249], we fitted these measurements by combinations of logarithms and polynomials in $x$ of the form

$$
\begin{equation*}
\mathcal{F}_{C}\left(x ; \kappa=0, k, \delta=0, g_{I}^{( \pm)}=1\right)=\sum_{n=0}^{n_{\max }} P_{n}^{(m)}(x, k) \log ^{n}(x), \quad P_{n}^{(m)}(x, k)=\sum_{n=0}^{m} a_{n}^{(k)} x^{n} \tag{63}
\end{equation*}
$$

where the upper limit $n_{\max }$ is determined by the power $-n_{\text {max }}$ of the leading pole in the Laurentexpansion (in $\epsilon$ ) of the integral. As for the degree of the polynomials we tried several simple choices ( $m=1,2,3$ ). We found that splitting the region of the parameter space into an asymptotic ( $0<x \leq$ $10^{-4}$ ) and a non-asymptotic ( $10^{-4}<x \leq 1$ ) region, we could provide a fit with $m=2$ that approximates the analytic result within relative difference few times $10^{-4}$. The loss of relative precision is associated with phase space points where the function changes sign, and its numerical value is close to zero (around $x=0.2$ ).

In Fig. 8 we show the approximate function $\mathcal{F}_{C}\left(x ; \alpha_{0}, d_{0}, 0,-1,0,1\right)$ together with the 'measurements', which coincide with the known exact analytic result to at least six digit accuracy. We find very good agreement, which is characterized by the ratio of the two values in the lower panels. In Fig. 8 b we show the approximate function for $\alpha_{0}=0.1$ and $d_{0}=3-3 \epsilon$ together with the corresponding 'measurements'. In this case the analytic results are not available.

Building on the experience gained in studying the one-parameter case, we worked out a similar strategy for the integrated subtraction term $\int_{2} \mathcal{C}_{i r, j s}^{(0,0)}$. The corresponding functions $C_{i r, j s}^{(0,0)}$ can be ex-


Fig. 8: The fitted function $\mathcal{F}_{C}(x ; 0,-1,0,1)$ compared to the integral $\mathcal{I}(x ; 0,-1,0,1)$ at a) $\alpha_{0}=1$ and $d_{0}=3$, b) $\alpha_{0}=0.1$ and $d_{0}=3-3 \epsilon$.
pressed as combination of the integrals

$$
\begin{align*}
& \mathcal{I}_{2 C}\left(x_{i}, x_{j} ; \epsilon, \alpha_{0}, d_{0} ; k, l\right)=x_{i} x_{j} \int_{0}^{1} \mathrm{~d} \alpha \int_{0}^{1} \mathrm{~d} \beta \Theta\left(\alpha_{0}-\alpha-\beta\right) \\
& \quad \times(1-\alpha-\beta)^{2 d_{0}-2(1-\epsilon)} \alpha^{-1-\epsilon} \beta^{-1-\epsilon}\left(\alpha+(1-\alpha-\beta) x_{i}\right)^{-1-\epsilon}\left(\beta+(1-\alpha-\beta) x_{j}\right)^{-1-\epsilon} \\
& \quad \times \int_{0}^{1} \mathrm{~d} v v^{-\epsilon}(1-v)^{-\epsilon} \int_{0}^{1} \mathrm{~d} u u^{-\epsilon}(1-u)^{-\epsilon}\left(\frac{\alpha+(1-\alpha-\beta) x_{i} v}{2 \alpha+(1-\alpha-\beta) x_{i}}\right)^{k}\left(\frac{\beta+(1-\alpha-\beta) x_{j} u}{2 \beta+(1-\alpha-\beta) x_{j}}\right)^{l} . \tag{64}
\end{align*}
$$

We again run SecDec with $\alpha_{0}=0.1$ and $d_{0}=3-3 \epsilon$ at several hundred different values of the kinematic parameters to obtain the 'measurements'. To reach $10^{-7}$ relative precision for all such 'measurements' takes several hours on a single CPU. Then we fitted these 'measurements' with the function

$$
\begin{equation*}
\mathcal{F}_{2 C}\left(x_{i}, x_{j} ; k, l\right)=\sum_{n_{i}=0}^{n_{\max }} \sum_{n_{j}=0}^{n_{\max }-n_{i}} P_{n_{i}}^{(m)}\left(x_{i}, k, l\right) P_{n_{j}}^{(m)}\left(x_{j}, k, l\right) \log ^{n_{i}}\left(x_{i}\right) \log ^{n_{j}}\left(x_{j}\right) . \tag{65}
\end{equation*}
$$

We divide the parameter space $0<x_{i}, x_{j} \leq 1$ into four regions: (i) $0<x_{i}, x_{j} \leq 10^{-4}$, (ii) $0<x_{i} \leq$ $10^{-2}$ and $10^{-4}<x_{j} \leq 1$, (iii) $0<x_{j} \leq 10^{-2}$ and $10^{-4}<x_{i} \leq 1$, (iv) $10^{-2}<x_{i}, x_{j} \leq 1$. Using $m=2$, we are able to fit the original function $\mathcal{I}_{2 C}$ to per mille precision almost everywhere. The ratio of the fitted function $\mathcal{F}_{2 C}$ to the numerical evaluation of $\mathcal{I}_{2 C}$ is shown in Fig. 9 together whith the fitted function $\mathcal{F}_{2 C}$ itself.

## CONCLUSIONS

We have worked out a numerical procedure for providing simple approximations of the integrated subtraction terms of the NNLO subtraction scheme defined in Refs. [240, 241, 242, 243]. We use the publicly available program SecDec to compute the coefficients of the Laurent expansion of the necessary integrals to high numerical precision. We found that the integrals that depend on one or two kinematical invariants can be approximated with simple combinations of polynomials and logarithms. The precision of these approximations is usually at per mille or better.


Fig. 9: The ratio of the fitted function $\mathcal{F}_{2 C}\left(x_{i}, x_{j} ;-1, l\right)$ to the integral $\mathcal{I}_{2 C}\left(x_{i}, x_{j} ;-1, l\right)$. a) $\left.l=-1 \mathbf{b}\right)$ $l=0$ Also shown the fitted function $\mathcal{F}_{2 C}\left(x_{i}, x_{j} ;-1,-l\right)$.

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## Part III

## PARTON DISTRIBUTION FUNCTIONS

## 7. WHICH EXPERIMENTS CONSTRAIN THE GLUON PDF IN A GLOBAL QCD FIT? 9


#### Abstract

Based on computation of PDF-induced correlations, we identify the experiments in CTEQ and MSTW global QCD analyses that are sensitive to the gluon parton density in the proton. The Tevatron inclusive jet production at large momentum fractions $x$ and DIS charm quark production at moderately small $x$ show the strongest correlation with the gluon PDF. The strength of the PDF-induced correlation between the gluon PDF and inclusive (di)jet production data is different in the CTEQ and MSTW analyses.


### 7.1 Introduction

The parton distribution function (PDF) of gluons in a proton, $g(x, \mu)$, plays an important role in hadron collider phenomenology. It arises in cross sections for production of hadronic final states, massive scalar

[^199]

Fig. 10: CT10 and CTEQ 6.6 PDF uncertainty bands at $\mu=2 \mathrm{GeV}$ (left) and 100 GeV (right), taken from Ref. [255]. The CTEQ 6.6 best-fit PDFs and uncertainties are indicated by solid curves and hatched bands, while those of CT10 are indicated by dashed curves and dotted bands.
bosons, and hypothetical elementary particles, often in a combination with an overall normalization prefactor proportional to $\alpha_{s}$. The gluon distributions from CT10 [255] and CTEQ 6.6 [256] PDF sets are shown in Fig 10. The figure shows that the gluon PDF is constrained well by fitted experiments at the intermediate momentum fractions $x$, but the uncertainty grows in the region $x>0.1$. We may ask which experiments in the global fit impose the most significant constraints on the the gluon PDF. It is often said that the precise neutral-current DIS data provides the tightest constraints on the gluon PDF at $x$ of order $10^{-3}$, while inclusive jet production at the Tevatron plays the key role in constraining the gluon at $x>0.1$. However, the net PDF uncertainty reflects subtle interplay of numerous constraints imposed by QCD theory and multiple experiments, as well as various correlated uncertainties in experimental measurements. In this contribution, we identify the experiments with the strongest sensitivity to the gluon PDF by using a method of PDF-induced correlations that was developed in Refs. [256, 257, 258]. The analysis of correlations provides a systematic way to identify such experiments and also to establish specific ranges of $x$ and $Q$ where the correlations of the experimental data sets with the gluon PDF are the most pronounced.

### 7.2 Log-likelihood $\chi^{2}$ and PDF-induced correlations

The quality of theory description of an experimental data set can be quantified by the log-likelihood function $\chi^{2}$. Many high-energy physics experiments publish three kinds of measurement errors for each data point $i$ : the statistical error $\sigma_{i}$, uncorrelated systematic error $u_{i}$, and correlated systematic errors $\left\{\beta_{1 i}, \beta_{2 i}, \beta_{3 i} \ldots . \beta_{K i}\right\}$ of $K$ different types. To compare a theory prediction $T_{i}$ to the data value $D_{i}$ for a data point $i$, while accounting for all types of errors, the $\chi^{2}$ function can be constructed as [259, 260]

$$
\begin{equation*}
\chi^{2}=\sum_{\text {expt. }}\left[\sum_{i=1}^{N_{e}}\left(\frac{D_{i}-T_{i}(a)-\sum_{k=1}^{K} r_{k} \beta_{k i}}{\alpha_{i}^{2}}\right)^{2}+\sum_{k=1}^{K} r_{k}^{2}\right] \tag{66}
\end{equation*}
$$

where $\alpha_{i}^{2}=\sigma_{i}^{2}+u_{i}^{2}$ is the combined uncorrelated error; $r_{k}$ are random parameters describing each of $K$ correlated errors (each distributed according to the standard normal distribution); $N_{e}$ is the number of
the data points; and $K$ is the number of the sources of the correlated systematic errors.
Analytic minimization of the function (66) with respect to the correlated systematic parameters $r_{k}$ renders the following result [257, 259]:

$$
\begin{equation*}
\left.r_{k}\right|_{\text {best fit }}=\sum_{k^{\prime}=1}^{K} A_{k k^{\prime}}^{-1} B_{k^{\prime}}, \tag{67}
\end{equation*}
$$

where $A_{k k^{\prime}}$ and $B_{k}$ are given by

$$
\begin{equation*}
A_{k k^{\prime}}=\delta_{k k^{\prime}}+\sum_{i=1}^{N_{e}} \frac{\beta_{k i} \beta_{k^{\prime} i}}{\alpha_{i}^{2}}, \quad \text { and } \quad B_{k}=\sum_{i=1}^{N_{e}} \frac{\beta_{k i}\left(D_{i}-T_{i}\right)}{\alpha_{i}^{2}} . \tag{68}
\end{equation*}
$$

Substituting Eq. 67] into Eq. (66], we obtain a reduced $\chi^{2}$ function [257, 259],

$$
\begin{equation*}
\chi^{2}=\sum_{\text {expt. }}\left[\sum_{i=1}^{N_{e}} \frac{\left(D_{i}-T_{i}\right)^{2}}{\alpha_{i}^{2}}-\sum_{k, k^{\prime}=1}^{K} B_{k} A_{k k^{\prime}}^{-1} B_{k^{\prime}}\right] . \tag{69}
\end{equation*}
$$

In this function, the information about the systematic shifts in $r_{k}$ is included implicitly. Often, the influence of the correlated shifts on the PDFs is substantial.

Next, we wish to discuss correlations between PDF uncertainties of two variables, $X(\vec{a})$ and $Y(\vec{a})$, where $\vec{a}=\left\{a_{1}, a_{2}, \ldots, a_{N}\right\}$ is the vector of $N$ PDF parameters. The correlations can be computed either in the Hessian [256, 257, 258] or Monte-Carlo [261] approaches. In this note we will adopt the Hessian approach.

A symmetric PDF uncertainty $\Delta X$ corresponds to the maximal variation of $X$ for all combinations of PDF parameters that lie within the tolerance hypersphere $\Delta \chi^{2} \leq T^{2}$. This uncertainty is given by

$$
\begin{equation*}
\Delta X=\frac{1}{2} \sqrt{\sum_{i=1}^{N}\left[X_{i}^{+}-X_{i}^{-}\right]^{2}} \tag{70}
\end{equation*}
$$

in terms of the value $X_{0}$ of $X$ obtained with the central PDF set, and values $X_{i}^{+}$and $X_{i}^{-}$of $X$ obtained for maximal positive and negative displacements of each orthonormal PDF parameter $a_{i}$ within the tolerance hypersphere. The same "master equation" defines $\Delta Y$, the PDF uncertainty of the variable $Y$.

In the linear approximation, the pairs of values of $X$ and $Y$ that are allowed within the PDF uncertainty correspond to the points inside an ellipse in the $X-Y$ plane. The boundary of the ellipse is parametrically described by

$$
\begin{align*}
& X=X_{0}+\Delta X \cos \theta  \tag{71}\\
& Y=Y_{0}+\Delta Y \cos (\theta+\varphi) \tag{72}
\end{align*}
$$

where the parameter $\theta$ varies between 0 and $2 \pi$, and the relative phase angle $\varphi$ is a function of $X_{i}^{ \pm}$and $Y_{i}^{ \pm}$. The PDF uncertainties $\Delta X$ and $\Delta Y$ are calculated according to Eq. 70). The angle $\varphi$ is included between the gradients $\vec{\nabla} X$ and $\vec{\nabla} Y$ of $X$ and $Y$ in the PDF parameter space. Its cosine,

$$
\begin{equation*}
\cos \varphi=\frac{\vec{\nabla} X \cdot \vec{\nabla} Y}{\Delta X \Delta Y}=\frac{1}{4 \Delta X \Delta Y} \sum_{i=1}^{N}\left(X_{i}^{(+)}-X_{i}^{(-)}\right)\left(Y_{i}^{(+)}-Y_{i}^{(-)}\right) \tag{73}
\end{equation*}
$$

quantifies the degree of similarity in the PDF dependence of $X$ and $Y$. If $X$ and $Y$ are strongly correlated (corresponding to $\cos \varphi \rightarrow 1$ ) or anti-correlated $(\cos \varphi \rightarrow-1)$, the PDF uncertainties of $X$ and $Y$ are driven by essentially the same combinations of PDF parameters. Conversely, the PDF dependence of $X$ is independent from the PDF dependence of $Y$ if $\cos \varphi \approx 0$.

### 7.3 Which experiments are sensitive to the gluon PDF?

If an experimental cross section $\sigma$ strongly constrains a PDF $f_{a}(x, Q)$ for some combination of $x$ and $Q$, we expect that Eq. $\sqrt{73} \mid$ returns $|\cos \varphi|$ close to unity when using $X=f_{a / A}(x, Q)$ and $Y=\sigma$. If the experimental data set includes several data points, we can use $Y=\chi^{2}$. The strength of the constraint on the PDF from this experiment is determined by $|\cos \varphi|$ and the magnitude of $\chi^{2}$. In the majority of the fitted experiments, $\chi^{2} / N_{e}$ is close to 1 , so that $|\cos \varphi|$ tends to be more important for distinguishing between the sensitivities of the experiments than the magnitude of $\chi^{2}$.

Following this approach, we compute $\cos \varphi$ between the NLO gluon PDF $g(x, Q)$ in various $x$ ranges (for $Q^{2}=10 \mathrm{GeV}^{2}$ ), and $\chi^{2}$ for typical experimental data sets that are used in the PDF analysis. In this study, we compute $\cos \varphi$ for the experiments from the CT10 analysis that are listed in Table 4 . In the figures, we refer to each experiment by its numerical ID that is shown in the left column of Table 4 .

The $\cos \varphi$ values between the gluon PDF at a given $x$ value and $\chi^{2}$ for each experiment are plotted as two-dimensional contour plots for CT10 NLO PDFs [255] in the left panel of Fig. [11, and for MSTW' 08 NLO PDFs [262] in the right panel. The horizontal axis indicates the range of $x$ in $g(x, Q)$. The vertical axis indicates the ID of the experiment. At the bottom of the figure, we show the color legend adopted to draw the contour plots. The color legend is chosen so as to emphasize only cells with large correlation ( $\cos \varphi>0.5$, dark yellow-red colors) or large anticorrelation ( $\cos \varphi<-0.5$, blue colors). The regions with $|\cos \varphi|<0.5$ are filled with a light-yellow color. The $\chi^{2}$ values for each data set are computed according to Eqs. (66) and (69) using the CTEQ fitting code for both CT10 and MSTW PDF sets.

Visual inspection of two panels of Fig. 11 reveals both similarities and differences in the pattern of correlations of the gluon PDF in the CT10 and MSTW PDF sets. In the case of the CT10 PDF (left panel), the gluon PDF has a pronounced anti-correlation (blue spots) with HERA charm and bottom SIDIS production data sets (experiments $140,143,145,156,157$ ) at $x<0.1$, as well as with Tevatron inclusive jet production data sets (experiments $504,505,514$, and 515) at $x>0.05$. Some correlations (brown and red spots) are also observed, but they are not as pronounced as the anti-correlations. Weaker (anti-)correlations can be noticed with the NMC $F_{2}^{p}$, CDHSW $F_{2}^{p}$, and E605 pp Drell-Yan process data, corresponding to experiments 103, 108, and 201.

While the gluon PDF of the MSTW'08 set (right panel of Fig. 11) also shows an (anti-)correlation with the heavy-quark DIS and jet production data, the overall pattern of the correlations is somewhat different from the CT10 case. Here, the gluon PDF is mostly correlated with high- $x$ jet production (experiments 504, 505,514, and 515), while it is either correlated or anti-correlated with heavy-quark DIS experiments (experiments 140, 143, 145, 156, 157). In addition, we observe significant (anti-)correlations with the combined HERA DIS data set ( $\mathrm{ID}=159$ ) and fixed-target DIS experiments ( $\mathrm{ID}=101-124$ ) that are not seen in the CT10 panel.

We now turn to the correlations of the gluon and $u$-quark PDFs with $\chi^{2}$ values in individual bins of Tevatron inclusive jet and dijet production data. For this purpose, we represent $\chi^{2}$ for one experimental data set in Eq. 69 as a sum of contributions $\chi_{i}^{2}$ from individual data points $i$ :

$$
\begin{equation*}
\chi^{2}=\sum_{i=1}^{N_{e}} \chi_{i}^{2}, \tag{74}
\end{equation*}
$$

where

$$
\begin{equation*}
\chi_{i}^{2}=\frac{D_{i}-T_{i}}{\alpha_{i}} \sum_{j=1}^{N_{e}}\left\{\delta_{i j}-\frac{D_{j}-T_{j}}{\alpha_{j}} \sum_{k, k^{\prime}=1}^{K} \frac{\beta_{k i}}{\alpha_{i}} A_{k k^{\prime}}^{-1} \frac{\beta_{k^{\prime} j}}{\alpha_{j}}\right\} . \tag{75}
\end{equation*}
$$

Each contribution $\chi_{i}^{2}$ accounts for the effect of correlated systematic shifts through the term that includes $A_{k k^{\prime}}^{-1}$ on the right-hand side of Eq. 75 . Again, the constraining power of each point is determined both


Fig. 11: Correlation between the gluon distribution from CT10 NLO (left) and MSTW2008 NLO (right) PDF sets and $\chi^{2}$ for the experiments used in the CT10 global QCD analysis. The color of each cell indicates the value of $\cos \varphi$ according to the included legend. The ID's of individual experiments are listed in Table 4

| ID | Experimental data set |
| :---: | :---: |
| 159 | Combined HERA1 NC and CC DIS [263] |
| 101 | BCDMS $F_{2}^{p}$ [264] |
| 102 | BCDMS $F_{2}^{d}$ [265] |
| 103 | NMC $F_{2}^{p}$ [266] |
| 104 | NMC $F_{2}^{d} / F_{2}^{p}$ [266] |
| 108 | CDHSW $F_{2}^{p}$ [267] |
| 109 | CDHSW $F_{3}^{p}$ [267] |
| 110 | CCFR $F_{2}^{p}$ [268] |
| 111 | CCFR $x F_{3}^{p}$ [269] |
| 124 | NuTeV neutrino dimuon SIDIS [270] |
| 125 | NuTeV antineutrino dimuon SIDIS [270] |
| 126 | CCFR neutrino dimuon SIDIS [271] |
| 127 | CCFR antineutrino dimuon SIDIS [271] |
| 140 | H1 $F_{2}^{c}$ [272] |
| 143 | H1 $\sigma_{r}^{c}$ for $c \bar{c}$ [273, 274] |
| 145 | H1 $\sigma_{r}^{b}$ for $b \bar{b}$ [273, 274] |
| 156 | ZEUS $F_{2}^{c}$ [275] |
| 157 | ZEUS $F_{2}^{c}$ [276] |
| 201 | E605 Drell-Yan process, $\sigma(p A)$ [277] |
| 203 | E866 Drell Yan process, $\sigma(p d) /(2 \sigma(p p))$ [278] |
| 204 | E866 Drell-Yan process, $\sigma(p p)$ [279] |
| 225 | CDF Run-1 $W$ charge asymmetry [280] |
| 227 | CDF Run-2 $W$ charge asymmetry [281] |
| 231-234 | DØ Run-2 W charge asymmetry [282] |
| 260 | DØ Run-2 Z rapidity distribution [283] |
| 261 | CDF Run-2 Z rapidity distribution [284] |
| 504 | CDF Run-2 inclusive jet production [285] |
| 505 | CDF Run-1 inclusive central jet production [286] |
| 514 | DØ Run-2 inclusive jet production [287] |
| 515 | DØ Run-1 inclusive jet production [288] |

Table 4: Experimental data sets examined in this analysis.


Fig. 12: Correlation cosine between $\chi_{i}^{2}$ in each $p_{T}$ bin from D $\emptyset$ Run- 2 inclusive jet production and gluon and $u$ quark distributions from CT10 and MSTW 2008 NLO sets. The horizontal axis refers to the $x$ value in the PDF. The vertical axis indicates the numerical ID of the experimental bin for which $\chi^{2}$ is computed. The ID for each bin is indicated as $100 i_{y}+i_{p_{T}}$, where $i_{y}=1, \ldots 6$ and $i_{p_{T}}$ are the ID's of the corresponding rapidity interval and the $p_{T}$ interval, respectively.


Fig. 13: Correlation cosine between $\chi_{i}^{2}$ in each $m_{j j}$ bin from D $\emptyset$ Run-2 dijet production and gluon and $u$ quark distributions from CT10 and MSTW 2008 NLO sets. The horizontal axis refers to the $x$ value in the PDF. The vertical axis indicates the numerical ID of the experimental bin for which $\chi^{2}$ is computed. The ID for each bin is indicated as $100 i_{y_{\max }}+i_{m_{j j}}$, where $i_{y_{\max }}=1, . ., 6$ and $i_{m_{j j}}$ are the ID's of the corresponding intervals in $y_{\max }$ and $m_{j j}$, respectively.
by the value of $|\cos \varphi|$ and the magnitude of $\chi_{i}^{2}$, with the latter being comparable to unity for the majority of the data points.

For D $\emptyset$ Run-2 single-inclusive jet cross sections [287], we plot the $\cos \varphi$ values for the gluon and $u$-quark PDFs, with $\chi_{i}^{2}$ computed for each bin of the jet's transverse momentum $p_{T}$ and rapidity $y$. The resulting contour plots are shown in Fig. 12. Similarly, for DØ Run-2 dijet cross sections [289], Fig. 13 shows the contour plots of $\cos \varphi$ for $\chi_{i}^{2}$ in the bins of of dijet invariant mass $m_{j j}$ and maximal absolute rapidity $|y|=\max \left(\left|y_{1}\right|,\left|y_{2}\right|\right)$ of the dijets. In both figures, theory cross sections are computed at NLO (without threshold resummation corrections) with the FASTNLO code [290, 291], using the settings described in Section 13. The same color legend as in Fig. 11 is used. Similar patterns of correlations were found with the CDF Run-2 inclusive jet data (not shown).

The upper panels in both figures show $\cos \varphi$ for CT 10 NLO and MSTW' 08 NLO gluon PDFs. The correlated experimental errors modify the correlations by smearing the $\cos \varphi$ distribution. The pattern of $\cos \varphi$ indicates clearly that the (di)jet data are very sensitive to the gluon at $x$ above 0.01 . However, the correlation is weaker for the CT10 gluon PDF (left panel) then for MSTW'08 PDF (right panel), suggesting that the importance of the constraints on the gluon PDF from the jet data is not the same in two fits. In addition, the MSTW'08 $u$-quark PDF shows mild (anti-)correlation with both single-inclusive jet data and dijet data, as can be observed in the right lower panels in Figs. 12 and 13 . No pronounced (anti-)correlations with the $u$-quark PDF or other quark PDFs of physical flavors are observed for the CT10 set, shown in the lower left panels.

The contour plots confirm the expectation that the inclusive jet data play an important role in constraining the gluon PDF. While the constraints are strongest at $x>0.1$, they extend down to $x$ as low as 0.05 for both CT10 and MSTW sets, as can be observed in Figs. 12 and 13 . The gluon PDF is sensitive to constraints from heavy-quark semi-inclusive DIS production at even lower $x$ values, cf. Fig. 11. As the HERA data on heavy-quark DIS production continue to improve, it will play an increasingly important role in constraining the low- $x$ gluon density.

While the patterns of PDF-induced correlations are visually similar for the CT10 and MSTW'08 sets, they are not completely identical. Constraints on the gluon PDF from Tevatron jet production may not be as strong in the CT10 fit as in the MSTW'08 fit, according to Figs. 12 and 13 It remains to be investigated what causes the observed differences between CT10 and MSTW sets in the correlations involving the gluon PDF. Several features are different in these fits, including different heavy-quark DIS schemes, choice of experimental data sets, PDF parametrizations, and radiative contributions in theoretical cross sections. A combination of these effects may indirectly affect the strength of the constraints imposed on the gluon density by the collider jet data.

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## 8. PDF CONSTRAINTS FROM ELECTROWEAK VECTOR BOSON PRODUCTION AT THE LHC ${ }^{10}$


#### Abstract

We present a study of the impact of the recent $W$ and $Z$ measurements from ATLAS, CMS and LHCb on parton distribution functions. We show that the NNPDF2.1 NNLO predictions are consistent with all the new data, but that these provide significant further constraints on the light quarks and antiquarks


[^200]at medium and small- $x$. We conclude that these data already have the potential to play a useful role in future global PDF analyses.

### 8.1 LHC measurements sensitive to PDFs

The LHC has already provided an impressive set of measurements which are sensitive to parton distributions: inclusive jet and dijet data [292, 293, 294], electroweak vector boson production [295, 296, 297, 298, 299, 300] (both inclusive and in association with heavy quarks [301]) and direct photon production [302, 303]. The purpose of this contribution is to quantify the impact on PDFs of a subset of these data, the $W$ and $Z$ inclusive production measurements. In this first section we will review the status of LHC data relevant for PDF determination and then in the next section we will study how the $W, Z$ data impact on the NNPDF analysis.

Let's begin this short review of LHC data with electroweak vector boson production. ATLAS has measured the $W$ lepton and $Z$ rapidity distributions using the 2010 data ( $36 \mathrm{pb}^{-1}$ ) and determined the full covariance matrix of correlated experimental uncertainties [295]. This measurement supersedes the original muon asymmetry measurement from $W$ decays [296], for which the covariance matrix was not available. The CMS collaboration has presented a preliminary measurement of the muon asymmetry with 2011 data ( $234 \mathrm{pb}^{-1}$ ) [297] which supersedes the 2010 data [298]. In addition it has presented a measurement of the normalized $Z$ rapidity distribution using 2010 data [299]. In neither of these two measurements has the full covariance matrix been made available. Finally, the LHCb Collaboration has presented preliminary results for the $Z$ rapidity distribution, $W$ lepton asymmetry and W lepton charge ratio using 2010 data [300].

| Data Set | Ref. | $N_{\text {dat }}$ | $\left[\eta_{\text {min }}, \eta_{\text {max }}\right]$ | $\left\langle\sigma_{\text {stat }}\right\rangle(\%)$ | $\left\langle\sigma_{\text {sys }}\right\rangle$ (\%) | $\left\langle\sigma_{\text {norm }}\right\rangle$ (\%) |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| ATLAS W,Z $36 \mathrm{pb}^{-1}$ | [295] | 30 | [0, 3.2] | 1.9 | 1.7 | 3.4 |
| ATLAS $W^{+} 36 \mathrm{pb}^{-1}$ | [295] | 11 | [0, 2.4] | 1.4 | 1.3 | 3.4 |
| ATLAS $W^{-} 36 \mathrm{pb}^{-1}$ | [295] | 11 | [0, 2.4] | 1.6 | 1.4 | 3.4 |
| ATLAS $Z 36 \mathrm{pb}^{-1}$ | [295] | 8 | [0, 3.2] | 2.8 | 2.4 | 3.4 |
| CMS $Z$ rapidity $36 \mathrm{pb}^{-1}$ | [299] | 35 | [0, 3.6] | 12.3 | - | 0 |
| CMS muon asymmetry $234 \mathrm{pb}^{-1}$ | [297] | 11 | [0, 2.4] | 1.7 | 3.1 | 0 |
| LHCb $Z$ rapidity $36 \mathrm{pb}^{-1}$ | [300] | 5 | [2, 4.5] | 20 | 5 | 3.4 |
| LHCb $W$ lepton asymmetry $36 \mathrm{pb}^{-1}$ | [300] | 5 | [2, 4.5] | 16 | 21 | 0 |

Table 5: The number of data points, kinematical coverage and average statistical, systematic and normalization percentage uncertainties for each of the experimental LHC $W$ and $Z$ datasets considered in the present analysis. For the CMS $Z$ rapidity data, the systematic uncertainty is included in the statistical uncertainty: there is no normalization uncertainty because these data are normalised to the total cross-section.

The kinematical coverage of each of the various LHC $W$ and $Z$ dataset with the corresponding average experimental uncertainties for each dataset are summarized in Table5. As we can see the LHC electroweak data span a large range in rapidity up to $\eta=4.5$. Each of the three processes considered, $W^{+}, W^{-}$and $Z$ is sensitive to different partonic subprocesses.

There are other LHC datasets potentially sensitive to PDFs. Jet production from the Tevatron has been a very important measurement not only to constrain the gluon at high $x$, but in determining the strong coupling from a global PDF analysis [304, 305]. Similar constraints are expected from the LHC jet data, extended into a wider kinematical range. From the $2010\left(36 \mathrm{pb}^{-1}\right)$ dataset inclusive jet and dijet production has been measured by both CMS [292, 293] and ATLAS [294], however only for ATLAS is the full experimental covariance matrix available. The LHC inclusive jet data can be treated within a global analysis framework using tools like FastNLO or APPLgrid [306]. Since the full NNLO corrections to the inclusive jet production are unknown, jet data in a NNLO analysis can be included only within some approximation: for example with NNLO PDF evolution and coupling running but with NLO matrix elements, or else with NLO matrix elements supplemented with Sudakov estimates of the

NNLO corrections. Another LHC measurement that has the potential to constrain the gluon PDFs is prompt photon production from ATLAS [302] and CMS [303]: its consistency with NLO QCD and their impact on the NNPDF2.1 PDFs will be discussed in detail in Ref. [307].

### 8.2 PDF constraints from LHC $W$ and $Z$

Until recently all available NNPDF sets [308, 309, 261, 310, 311, 312, 313] were based on non-LHC data. NNPDF2.2 [314] was the first set to include LHC data, the $W$ lepton asymmetry from ATLAS and CMS [298, 296]. However now these two datasets are outdated, the first because now the full correlation matrix of the $W$ and $Z$ lepton distributions is available, and the second because data from higher luminosities is also available. So we have chosen to continue to use as our baseline the NNPDF2.1 NNLO set.

We now study the impact of the latest LHC $W$ and $Z$ data on the NNPDF parton distributions. All our theoretical NNLO predictions will be computed with DYNNLO [315] with the same cuts and settings as in the respective measurements. The impact of the new data will be quantified using the reweighting method of Refs. [316, 314] applied to the $N_{\text {rep }}=1000$ replicas of the NNPDF2.1 NNLO set.

To begin with, we have computed the $\chi^{2}$ for each of the datasets in Table 5 for the most recent NNLO PDF sets currently available on LHAPDF: NNPDF2.1, MSTW08 [262], ABKM09 [317], HERAPDF1.5 [318] and JR09 [319]. When available, we use the full experimental covariance matrix. Normalization uncertainties are included using the $t_{0}$ method [320]. This is important specially for the treatment of the ATLAS differential distributions where normalization uncertainties are comparable to the statistical and systematic uncertainties (See Table 5).

The results are summarized in Table 6. For the ATLAS $W$ and $Z$ lepton distributions we show the results both for the total dataset and the individual subsets, where in the latter case cross-correlations between subsets have been neglected. In all cases the theoretical NNLO predictions have been obtained with DYNNLO as discussed above. We can see that none of these PDF sets describes the ATLAS and CMS data perfectly, although NNPDF2.1 and HERAPDF1.5 give probably the best description, while ABKM09 and JR09 are significantly worse. All five sets give a reasonable description of the LHCb data within their large uncertainties.

| Dataset | $\chi^{2}$ NNPDF2.1 | $\chi^{2}$ MSTW08 | $\chi^{2}$ ABKM09 | $\chi^{2}$ JR09 | $\chi^{2}$ HERAPDF1.5 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| ATLAS | 2.7 | 3.6 | 3.6 | 5.0 | 2.0 |
| ATLAS $W^{+} 36 \mathrm{pb}^{-1}$ | 5.7 | 6.5 | 11.4 | 5.4 | 5.3 |
| ATLAS $W^{-} 36 \mathrm{pb}^{-1}$ | 2.5 | 4.1 | 5.4 | 8.0 | 6.4 |
| ATLAS $Z 36 \mathrm{pb}^{-1}$ | 1.8 | 3.7 | 4.2 | 6.5 | 2.9 |
| CMS | 2.0 | 3.0 | 2.8 | 3.6 | 2.8 |
| CMS $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.9 | 2.9 | 2.7 | 2.0 | 3.0 |
| CMS muon asymmetry $234 \mathrm{pb}^{-1}$ | 2.0 | 3.4 | 3.0 | 8.7 | 2.1 |
| LHCb | 0.8 | 0.7 | 1.2 | 0.4 | 0.6 |
| LHCb $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.1 | 0.7 | 0.8 | 0.6 | 0.8 |
| LHCb $W$ lepton asymmetry $36 \mathrm{pb}^{-1}$ | 0.5 | 0.6 | 1.6 | 0.2 | 0.5 |

Table 6: Comparison between LHC $W$ and $Z$ data and the most recent NNLO PDFs. For each PDF set we provide the $\chi^{2} / d o f$ between data and theory predictions, computed using the $t_{0}$-method.

For the ATLAS data, we would like to emphasize the importance of properly taking into account the correlations between datasets, specially the normalization: the description of the individual $W^{+}$, $W^{-}$and $Z$ datasets is always worse than the overall description because of these cross-correlations. For the CMS $Z$ rapidity distribution we find that the fixed order NNLO description seems rather worse than the NLO+LL prediction implemented in POWHEG [299]: the origin of this difference should be investigated in future studies.

We now discuss the impact of these LHC EW data into the NNPDF2.1 NNLO PDFs [313]. In Table 7 we summarize the initial $\chi^{2}$ for each dataset, the $\chi^{2}$ after reweighting, $\chi_{\mathrm{rw}}^{2}$. We find excellent agreement with all the LHC electroweak measurements after reweighting. Some comparisons between data and theory for a selected observables are shown in Fig. 14. From top to bottom we show the comparison with ATLAS, CMS and LHCb data. In each case we have included all the most updated electroweak datasets from each collaboration.

In Table 7 we also show the effective number of replicas left after the reweighting, defined as in Ref. [316] using the Shannon entropy,

$$
\begin{equation*}
N_{\text {eff }} \equiv \exp \left\{\frac{1}{N_{\text {rep }}} \sum_{k=1}^{N_{\text {rep }}} w_{k} \ln \left(N_{\text {rep }} / w_{k}\right)\right\} \tag{76}
\end{equation*}
$$

In each case we have performed the reweighting separately for each of the experimental datasets individually, for the combined datasets from each experiment, and finally with all three combined together.

| Dataset | $\chi^{2}$ | $\chi_{\mathrm{rw}}^{2}$ | $N_{\text {eff }}$ |
| :---: | :---: | :---: | :---: |
| ATLAS | 2.7 | 1.2 | 16 |
| ATLAS $W^{+} 36 \mathrm{pb}^{-1}$ | 5.7 | 1.5 | 17 |
| ATLAS $W^{-} 36 \mathrm{pb}^{-1}$ | 2.5 | 1.0 | 205 |
| ATLAS $Z 36 \mathrm{pb}^{-1}$ | 1.8 | 1.1 | 581 |
| CMS | 2.0 | 1.2 | 56 |
| CMS $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.9 | 1.4 | 223 |
| CMS muon asymmetry $234 \mathrm{pb}^{-1}$ | 2.0 | 0.4 | 200 |
| LHCb | 0.8 | 0.8 | 972 |
| LHCb $Z$ rapidity $36 \mathrm{pb}^{-1}$ | 1.1 | 1.0 | 962 |
| LHCb $W$ lepton asymmetry $36 \mathrm{pb}^{-1}$ | 0.8 | 0.5 | 961 |
| All data combined | 2.1 | 1.2 | 4 |

Table 7: The impact of LHC electroweak measurements on the NNPDF2.1 NNLO PDFs. For each dataset we show the initial $\chi^{2}$, the $\chi^{2}$ after reweighting these particular dataset and the effective number of replicas $N_{\text {eff }}$ in this case. We show both the results for individual datasets as well as for the combined impact of all datasets within the same experiment. All the results have been computed starting with $N_{\text {rep }}=1000$ replicas.

When all the datasets are taken together, the initial $\chi^{2}=2.1$, already quite reasonable is reduced down to $\chi_{\mathrm{rw}}^{2}=1.2$, thus obtaining a very good overall description of all the most recent LHC electroweak data. The effective number of replicas for all combined datasets is only $N_{\text {eff }}=4$ however: from this we conclude that to determine the combined impact of these data on PDFs would require many more replicas (around 25,000 in fact, to obtain reasonable statistical accuracy), or, more practically, a new fit. Note that the fact that the total effective number of replicas for the whole dataset is rather smaller than that of any individual subset confirms their mutual compatibility and the lack of any appreciable tension. Comparing the effective number of replicas for the individual datasets, the most constraining data are the ATLAS $W$ and $Z$ distributions, specially the very precise $W^{+}$data. On the other hand the LHCb data have a rather small impact.

Let us now examine how various PDFs change when new experiments are added. In particular we show in Fig. 15 the NNPDF2.1 NNLO $d\left(x, Q^{2}\right)$ and $\bar{u}\left(x, Q^{2}\right)$ PDFs at $Q^{2}=M_{W}^{2}$ as ratios to the central value before including the new data. As described above, we put together all the data from a given experiment. As can be seen, the ATLAS data give a moderate reduction in PDF uncertainties, and a somewhat softer small- $x$ sea quarks, although the old and new PDFs agree at the 1 -sigma level. For CMS the central values for the old and new PDFs are unchanged with a moderate error reduction at medium- $x$. Finally, for LHCb the PDF uncertainties are almost unaffected, due to the low constraining power of these datasets.


Fig. 14: Comparison between data and theory before and after reweighting for NNPDF2.1 NNLO compared to the various LHC EW datasets considered. From top to bottom we show comparisons with ATLAS ( $W^{+}$lepton $Z$ rapidity distributions), CMS ( $W$ lepton asymmetry and $Z$ rapidity distribution) and LHCb data (same as CMS). For the ATLAS data the error bars include statistical and systematic uncertaintes, but not the normalization uncertainties.

### 8.3 Conclusions

In this contribution we have quantified the impact of the most updated LHC electroweak data on the NNPDF2.1 NNLO parton distributions. NNPDF2.1 provides a reasonable description of all these datasets even before their impact on the PDFs is included. We find that all the datasets are mutually consistent, with no obvious tensions. The PDF uncertainties for the light quarks and antiquarks at medium and small- $x$ are moderately reduced. The ATLAS $W, Z$ data seem to prefer a softer small- $x$ sea. It is clear from our results that the LHC $W$ and $Z$ data should play an important part in any future PDF global fit.

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Fig. 15: Comparison between the NNPDF2.1 NNLO parton distributions before and after reweighting with the various LHC EW datasets considered. From top to bottom: ATLAS, CMS and LHCb data, where the left column we show the ratio of the $d$ quark PDF and in the right column the ratio of the $\bar{u}$ quark PDF to their central values before reweighting.


Fig. 16: $F_{L}$ vs. $Q^{2}$ for the HERA combined measurements from H 1 and ZEUS [321].

## 9. HEAVY QUARK PRODUCTION IN THE ACOT SCHEME AT NNLO AND $\mathbf{N}^{3} \mathbf{L O}^{11}$


#### Abstract

We extend the ACOT scheme for heavy quark production to NNLO and $\mathrm{N}^{3} \mathrm{LO}$ for the structure functions $F_{2}$ and $F_{L}$ in deep-inelastic scattering (DIS). We use the fully massive ACOT scheme up to NLO, and estimate the dominant heavy quark mass effects at the higher orders using the massless Wilson coefficients together with a generalized slow-rescaling prescription. We present results for $F_{2}$ and $F_{L}$ showing the effect of the higher orders and the contributions from the heavy flavors.


### 9.1 INTRODUCTION

The production of heavy quarks in high energy processes has become an increasingly important subject of study both theoretically and experimentally. The theory of heavy quark production in perturbative Quantum Chromodynamics ( pQCD ) is more challenging than that of light parton (jet) production because of the additional heavy quark mass scale. The correct theory must properly take into account the changing role of the heavy quark over the full kinematic range of the relevant process from the threshold region (where the quark behaves like a typical "heavy particle") to the asymptotic region (where the same quark behaves effectively like a parton, similar to the well known light quarks $\{u, d, s\}$ ).

With the ever-increasing precision of experimental data and the progression of theoretical calculations and parton distribution function (PDF) evolution to next-to-next-to-leading order (NNLO) of QCD, there is a clear need to implement the heavy quark schemes at this order and beyond. The most important case is arguably the heavy quark treatment in inclusive deep-inelastic scattering (DIS) since the very precise HERA data for DIS structure functions and cross sections form the backbone of any modern global analysis of PDFs. Here, the heavy quark structure functions contribute up to $30 \%$ or $40 \%$ to the inclusive structure functions at small momentum fractions $x$. Extending the heavy quark schemes to higher orders is relevant for extracting precision PDFs, and hence for accurate predictions of observables at the LHC.

An example where higher order corrections are particularly important is the longitudinal structure function $F_{L}$ in DIS. The leading order $\mathcal{O}\left(\alpha_{s}^{0}\right)$ contributions to this structure function vanishes for massless quarks due to helicity conservation (Callan-Gross relation). Since the first unsuppressed contribution to $F_{L}$ is at next-to-leading order, the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ corrections are more important than for $F_{2}$. In Fig. 16 we show the preliminary results for the $F_{L}$ measurement from the H1 and ZEUS experiments [321]. In Fig. 17 displays sample Feynman diagrams at the various orders. Producing an accurate

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Fig. 17: Example Feynman diagrams contributing to DIS heavy quark production (from left): LO $\mathcal{O}\left(\alpha_{S}^{0}\right)$ quark-boson scattering $Q V \rightarrow Q$, NLO $\mathcal{O}\left(\alpha_{S}^{1}\right)$ boson-gluon scattering $g V \rightarrow Q \bar{Q}$, NNLO $\mathcal{O}\left(\alpha_{S}^{2}\right)$ boson-gluon scattering $g V \rightarrow g Q \bar{Q}$ and $\mathrm{N}^{3} \mathrm{LO} \mathcal{O}\left(\alpha_{S}^{3}\right)$ boson-gluon scattering $g V \rightarrow g g Q \bar{Q}$.
prediction for $F_{L}$ is a challenge, particularly in the region of low $Q^{2}$ and small $x$.
In this paper, we will briefly outline the method we used to incorporate the higher order terms, the key elements of the ACOT scheme, and the treatment of the heavy quark masses. We then present results for the $F_{2}$ and $F_{L}$ neutral current DIS structure functions.

### 9.2 THE ACOT SCHEME AND ITS EXTENSION BEYOND NLO



Fig. 18: Comparison of schemes for $F_{2}^{c}$ at $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number Scheme (FFNS), and Zero-Mass Variable-Flavor-Number-Scheme (ZM-VFNS). The ACOT and S-ACOT results are virtually identical.

The ACOT scheme [322, 323] is based upon the factorization theorem for heavy quarks[324]; hence, it is valid at any order of perturbation theory. The factorization proof ensures that the ACOT scheme can be applied throughout the full kinematic regime, and that there is a smooth transition from a massless result $(m=0)$ to the heavy-mass decoupling limit $(m \rightarrow \infty)$.

In the limit where the quark $Q$ of mass $m$ is relatively heavy compared to the characteristic energy scale ( $\mu \lesssim m$ ), the ACOT result naturally reduces to the Fixed-Flavor-Number-Scheme (FFNS). In the FFNS, the heavy quark is treated as being extrinsic to the hadron, and there is no corresponding heavy quark PDF, $f_{Q}(x, \mu)=0$. Conversely, in the limit where the quark mass is relatively light $(\mu \gtrsim m)$, the ACOT result reduces to the $\overline{M S}$ Zero-Mass Variable-Flavor-Number-Scheme (ZM-VFNS) exactlywithout any finite renormalizations. In this limit, the quark mass $m$ no longer plays any dynamical role; it serves purely as a regulator. This feature is presented in Fig. 18 where we can see that the ACOT scheme precisely matches the results of the FFNS and ZM-VFNS schemes in their respective limits.

Additionally Fig. 18 shows the results obtained within the Simplified-ACOT scheme (SACOT) [325]. The S-ACOT scheme drops the heavy quark mass dependence for the hard-scattering


Fig. 19: $F_{L}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right). The three lines show the mass effects via the scaling variable: $n=\{0,1,2\}$, (Red, Green, Blue). We observe the effect of the $n$-scaling is negligible except for small $x$ and $Q$ values.
processes with incoming heavy quarks or with internal on-shell cuts on a heavy quark line. The S-ACOT scheme is not an approximation; it is an exact renormalization scheme, extensible to all orders. Note, the ACOT and S-ACOT results agree throughout the kinematic region.

### 9.21 Beyond NLO

While there is no conceptual difficulty with extending the ACOT scheme beyond NLO, the fully massive Wilson coefficients have yet to be computed ${ }^{[12}$ However massless calculations of NNLO and even $\mathrm{N}^{3} \mathrm{LO}$ for $F_{2}$ and $F_{L}$ structure functions are available $\sqrt{13}$

The question is: can we use these results, together with the knowledge that ACOT reduces to the massless $\overline{M S}$ (ZM-VFNS) for $m \rightarrow 0$, to estimate mass effects at NNLO and $\mathrm{N}^{3} \mathrm{LO}$ ? Obviously we cannot restore the fully massive ACOT result from the massless limit, but we can try to extract the dominant higher order contributions. There are two ways in which mass effects enter the calculation. The first is "dynamically" through the mass dependent Wilson coefficients. The second is "kinematically" via the restricted phase space. Comparisons using the fully massive results at NLO suggest that the kinematic mass effects are dominant, and that much of this dependence can be obtained with a rescaling of the Bjorken $x$ variable. We introduce a generalized rescaling $x \rightarrow x\left[1+(n m / Q)^{2}\right]$ where $n=0$ is the massless result, $n=1$ is the original Barnett[329] rescaling, and $n=2$ is the $\chi$-rescaling [330].

Thus, our strategy is as follows. We use the fully massive ACOT result to NLO [331], and add to this the massless NNLO and $\mathrm{N}^{3} \mathrm{LO}$ contributions using the generalized rescaling prescription. By varying $n$, we can investigate the influence of the kinematic mass in our results. We argue that the massless Wilson coefficients at NNLO and $\mathrm{N}^{3} \mathrm{LO}$, together with the generalized rescaling prescription provide a good approximation of the exact result. At worst, the error is of order $\alpha \alpha_{S}^{2} \times\left[m^{2} / Q^{2}\right]$, and comparative studies at NLO suggest the error is less. ${ }^{[14}$ For example, in Fig. 19 we display the results of $F_{L}$ for $n=\{0,1,2\}$. The effects of the detailed mass dependence is most noticeable for low $Q^{2}$ and small $x$. While the massless scaling result $(n=0)$ does deviate from the other curves, comparing the $n=1$ and $n=2$ curves we observe the details of the mass rescaling are relatively small. While this is not a proof ${ }_{[15}^{15}$ this result does give us confidence that the mass effects are under control.


Fig. 20: Fractional contribution for each quark structure function $F_{2, L}^{i}$ for each flavor $i=\{u, d, s, c, b\}$ for (a) $F_{2}^{i}$ and (b) $F_{L}^{i}$ vs. $Q$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$ (left to right) for the ACOT- $\chi$ scheme.

### 9.3 RESULTS

In Fig. 20 we display the fractional contributions to the structure functions $F_{2}$ and $F_{L}$. At larger values of $x$ and low $Q$, we observe that the heavy flavor contributions are minimal. For example, for $x=10^{-1}$, we see that the $u$-quark structure function $F^{u}$ comprises $\sim 80 \%$ of the total structure function. In contrast, at $x=10^{-5}$ and large $Q$ we see that the contributions of the $u$ and $c$ quarks are comparable (as they couple with a factor 4/9), and the $d$ and $s$ quarks contributions are comparable (as they couple with a factor $1 / 9$ ).

Figure 20 also shows how the $\chi$-rescaling introduces a damping of the heavy quark contributions as we move from large $Q^{2}$ values to smaller values. The $\chi$-rescaling ensures the heavy quarks $(c, b)$ are appropriately suppressed for low $Q^{2}$ scales.

In Fig. 21a we display the results for $F_{2}$ vs. $Q$ computed at various orders; the ratio to the $\mathrm{N}^{3} \mathrm{LO}$ result is displayed in Fig. 21b For large $x$ (c.f. $x=0.1$ ) we find the perturbative calculations are particularly stable. We see that the LO result is within $20 \%$ of the others at small $Q$, and within $5 \%$ at large $Q$. The NLO is within $2 \%$ at small $Q$, and indistinguishable from the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ for $Q$ values above $\sim 10 \mathrm{GeV}$. The NNLO and $\mathrm{N}^{3} \mathrm{LO}$ results are essentially identical throughout the kinematic range. For smaller $x$ values $\left(10^{-3}, 10^{-5}\right)$, the contributions of the higher order terms are slightly larger. Here, the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ coincide for $Q$ values above $\sim 5 \mathrm{GeV}$, but the NLO result can differ by $\sim 5 \%$ for low $Q^{2}$ scales.

In Fig. 22 we display the results for $F_{L}$ vs. $Q$ computed at various orders. In contrast to $F_{2}$, we find that NLO corrections are large; this is expected because the LO corrections to $F_{L}$ (which violate

[^202]
(a) $F_{2}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

(b) Ratio of $F_{2}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) compared to $F_{2}$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=$ $\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

Fig. 21: $F_{2}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$.
the Callan-Gross relation) are suppressed by $\left(m^{2} / Q^{2}\right)$ compared to the dominant gluon contributions which enter at NLO. Consequently, we observe that the LO result for $F_{L}$ receives large contributions from the higher order terms. Essentially, NLO is the first non-trivial order for $F_{L}$, and the subsequent contributions then converge. For example, at large $x$ (c.f. $x=0.1$ ) for $Q \sim 10 \mathrm{GeV}$ we find the NLO results yields $\sim 70 \%$ of the total, the NNLO is a $\sim 20 \%$ correction, and the $\mathrm{N}^{3} \mathrm{LO}$ is a $\sim 10 \%$ correction. For lower $x$ values $\left(10^{-3}, 10^{-5}\right.$ ) the convergence of the perturbative series improves, and the NLO results is within $\sim 10 \%$ of the $\mathrm{N}^{3} \mathrm{LO}$ result. Curiously, for $x=10^{-5}$ the NNLO and $\mathrm{N}^{3} \mathrm{LO}$ roughly compensate each other so that the NLO and the $\mathrm{N}^{3} \mathrm{LO}$ match quite closely for $Q \gtrsim 2 \mathrm{GeV}$.

### 9.4 CONCLUSIONS

We have computed the $F_{2}$ and $F_{L}$ structure functions in the ACOT scheme at NNLO and $\mathrm{N}^{3} \mathrm{LO}$. The full mass dependence is computed to NLO, and the dominant mass effects for the higher orders are approximated using a generalized rescaling; the details of this rescaling are demonstrated to be small. This allows us to make detailed predictions throughout the kinematic range investigated by HERA, and we obtain a reasonable estimate of the uncertainty due to the higher order mass effects. Together with the precise HERA data, these calculations facilitate accurate determination of the PDFs which are the foundation of the LHC calculations.

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(a) $F_{L}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) for fixed $x=\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

(b) Ratio of $F_{L}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$ (red, green, blue, cyan) compared to $F_{L}$ at $\mathrm{N}^{3} \mathrm{LO}$ for fixed $x=$ $\left\{10^{-1}, 10^{-3}, 10^{-5}\right\}$, (left to right) for ACOT- $\chi$ scheme.

Fig. 22: $F_{L}$ vs. $Q$ at $\left\{\mathrm{LO}, \mathrm{NLO}, \mathrm{NNLO}, \mathrm{N}^{3} \mathrm{LO}\right\}$.

## Part IV

## PHENOMENOLOGICAL STUDIES OF OBSERVABLES AND UNCERTAINTIES

## 10. FINITE-WIDTH EFFECTS IN TOP-QUARK PAIR PRODUCTION AND DECAY AT THE LHC ${ }^{16}$


#### Abstract

We investigate finite-top-width effects in top-quark pair production by comparing NLO QCD predictions for $\mathrm{pp} \rightarrow$ WWb $\overline{\mathrm{b}}$ to corresponding $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow$ WWb $\bar{b}$ results in the narrow-top-width limit. Finite-top-width effects, which result from non-resonant and off-shell contributions, are discussed in detail for the case of the inclusive cross section (with experimental cuts) and for selected differential observables in the di-lepton channel.


### 10.1 INTRODUCTION

Top-quark pair production at hadron colliders allows for key tests of the Standard Model and represents an omnipresent background to Higgs-boson and new-physics searches. The very large t $\bar{t}$ samples from the Tevatron and the LHC, and the steadily increasing systematic precision call for a continu-

[^203]ous improvement of theory predictions ${ }^{17}$ In this context, a reliable theoretical description of experimental cuts and exclusive $t \bar{t}$ observables, which depend on details of the $\mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ final state, requires higher-order calculations for top-pair production and decay. The first NLO QCD predictions for $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}+X[335,336$, 337] have been obtained in the narrow-top-width limit, an approximation where the $2 \rightarrow 4$ particle process is factorised into on-shell $t \bar{t}$ production and (anti)top decays, taking into account spin correlations. In this framework, it was shown that NLO QCD effects in top-quark decays have a significant impact on the kinematic properties of final-state leptons and b-jets [335, 336, 337], and play an important role for top-mass measurements at the LHC [338]. More recently, NLO QCD predictions for the complete $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}+X$ process became available [25, 23], which include all effects related to the finite top-quark width, i.e. on- and off-shell intermediate top quarks, non-resonant contributions, and their interference with resonant t $\bar{t}$ production. Besides new evidence for the importance of NLO corrections to $t \bar{t}$ production and decay, these studies provided a first quantitative assessment of finite-width effects in the inclusive cross section. Applying a numerical $\Gamma_{\mathrm{t}} \rightarrow 0$ extrapolation to the $\mathrm{NLO} \mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ predictions, it was found that finite-topwidth contributions to the WWbb cross section at the Tevatron and the LHC ( 7 TeV ) range from 0.2 to 1 percent [25, 23], which is perfectly consistent with the expected order of magnitude ( $\Gamma_{\mathrm{t}} / m_{\mathrm{t}} \simeq 0.9 \%$ ) of finite-top-width effects in inclusive observables.

In this study, we pursue the investigation of finite-top-width effects by means of a tuned comparison of the $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ NLO calculation of Ref. [25] against the narrow-top-width approximation of Ref. [336]. This permits us, for the first time, to investigate $\Gamma_{\mathrm{t}}$-effects in different phenomenologically interesting regions of the $\mathrm{WWb} \overline{\mathrm{b}}$ phase space, where large off-shell and non-resonant contributions cannot be excluded a priori as in the case of inclusive observables.

### 10.2 NARROW-TOP-WIDTH APPROXIMATION AND FINITE-WIDTH EFFECTS

Let us start by recalling the main features of the NLO QCD calculations of $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ in narrow-top-width approximation [336] and $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ with finite-top-width effects [25]. For brevity, we denote them as $t \bar{t}$ and WWbb calculations, respectively. Both calculations implement leptonic W-boson decays in spin-correlated narrow-W-width approximation.

In the narrow-top-width limit of Ref. [336], top-quark resonances are approximated by

$$
\begin{equation*}
\lim _{\Gamma_{\mathrm{t}} / m_{\mathrm{t}} \rightarrow 0} \frac{1}{\left(p_{\mathrm{t}}^{2}-m_{\mathrm{t}}^{2}\right)^{2}+m_{\mathrm{t}}^{2} \Gamma_{\mathrm{t}}^{2}}=\frac{\pi}{m_{\mathrm{t}} \Gamma_{\mathrm{t}}} \delta\left(p_{\mathrm{t}}^{2}-m_{\mathrm{t}}^{2}\right), \tag{77}
\end{equation*}
$$

with delta functions that enforce the on-shell conditions, $p_{\mathrm{t}}^{2}=m_{\mathrm{t}}^{2}$, and are accompanied by $1 / \Gamma_{\mathrm{t}}$ factors. Contributions of $\mathcal{O}\left(\Gamma_{\mathrm{t}} / m_{\mathrm{t}}\right)$, i.e. terms that do not involve two resonant top propagators, are systematically neglected. The differential $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$ cross section is factorised into the $\mathrm{pp} \rightarrow \mathrm{t} \mathrm{\bar{t}}$ cross section times $\mathrm{t} \rightarrow \mathrm{Wb}$ partial decay widths, $\mathrm{d} \sigma=\left(\mathrm{d} \sigma_{\mathrm{t} \overline{\mathrm{t}}} \mathrm{d} \Gamma_{\mathrm{t}} \mathrm{d} \Gamma_{\overline{\mathrm{t}}}\right) / \Gamma_{\mathrm{t}}^{2}$, taking into account top-quark spin correlations. The LO and NLO predictions can be schematically expressed as

$$
\begin{align*}
\mathrm{d} \sigma_{\mathrm{LO}} & =\Gamma_{\mathrm{t}, \mathrm{LO}}^{-2}\left(\mathrm{~d} \sigma_{\mathrm{tt}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{0}\right), \\
\mathrm{d} \sigma_{\mathrm{NLO}} & =\Gamma_{\mathrm{t}, \mathrm{NLO}}^{-2}\left[\left(\mathrm{~d} \sigma_{\mathrm{tt}}^{0}+\mathrm{d} \sigma_{\mathrm{t} \mathfrak{t}}^{1}\right) \mathrm{d} \Gamma_{\mathrm{t}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{0}+\mathrm{d} \sigma_{\mathrm{tt}}^{0}\left(\mathrm{~d} \Gamma_{\mathrm{t}}^{1} \mathrm{~d} \Gamma_{\mathrm{t}}^{0}+\mathrm{d} \Gamma_{\mathrm{t}}^{0} \mathrm{~d} \Gamma_{\mathrm{t}}^{1}\right)\right], \tag{78}
\end{align*}
$$

where the superscripts 0 and 1 indicate tree-level quantities and NLO corrections, respectively. The NLO prediction involves three terms, where the corrections are applied either to $\mathrm{d} \sigma_{\mathrm{tt}}$ or to one of the decays. All ingredients of $\mathrm{d} \sigma_{\mathrm{LO}}$ and $\mathrm{d} \sigma_{\mathrm{NLO}}$ have to be evaluated with input parameters at the corresponding perturbative order. In particular, LO and NLO predictions must be computed using $\Gamma_{\mathrm{t}, \mathrm{LO}}$ and $\Gamma_{\mathrm{t}, \mathrm{NLO}}$ decay widths, as indicated in $\left.\boxed{78}\right|^{18}$ This guarantees that-up to higher-order corrections-the integration over

[^204]the phase space of each top decay in (78) is consistent with the branching fraction
\[

$$
\begin{equation*}
\frac{\int \mathrm{d} \Gamma_{\mathrm{t} \rightarrow \mathrm{~b} l \nu}}{\Gamma_{\mathrm{t}}}=\frac{\Gamma_{\mathrm{t} \rightarrow \mathrm{~b} l \nu}}{\Gamma_{\mathrm{t}}}=\mathrm{BR}(\mathrm{t} \rightarrow \mathrm{~b} l \nu) . \tag{79}
\end{equation*}
$$

\]

In this context, let us point out that a consistent inclusion of finite-W-width corrections-both in the scattering amplitudes and the $\Gamma_{\mathrm{t}}$ input parameters-is expected to lead to doubly-suppressed effects. This is due to the fact that, in the $\Gamma_{\mathrm{t}} \rightarrow 0$ limit, $\mathcal{O}\left(\Gamma_{\mathrm{W}}\right)$ corrections to the numerator and denominator of the branching fraction (79) cancel. Finite-W-width corrections are thus expected to produce very small effects of $\mathcal{O}\left(\frac{\Gamma_{\mathrm{W}} \Gamma_{\mathrm{t}}}{M_{\mathrm{w}} m_{\mathrm{t}}}\right)$ in inclusive observables. This justifies the use of the narrow-W-width approximation in combination with finite-top-width contributions, which is the approach adopted in Ref. [25], although in kinematic regions where finite- $\Gamma_{\mathrm{t}}$ effects become large also finite-W-width corrections [23] might become non-negligible.

The calculation of Ref. [25] provides a full description of $\mathrm{pp} \rightarrow \mathrm{W}^{+} \mathrm{W}^{-} \mathrm{b} \overline{\mathrm{b}}$ at order $\mathcal{O}\left(\alpha_{\mathrm{S}}^{3} \alpha^{2}\right)$. The top-quark width is incorporated into the complex top mass, $\mu_{\mathrm{t}}^{2}=m_{\mathrm{t}}^{2}-\mathrm{i} m_{\mathrm{t}} \Gamma_{\mathrm{t}}$, in the complex-mass scheme [339]. In this way, off-shell-top contributions are consistently described by Breit-Wigner distributions. Besides contributions with two intermediate top resonances, also singly- and non-resonant diagrams are taken into account, including interferences. A few representative tree diagrams are shown in Fig 23. The NLO WWbb̄ predictions involve factorisable corrections to doubly-resonant diagrams, which provide the off-shell extension of NLO corrections in $t \bar{t}$ approximation (78). In addition, there are non-factorisable corrections, where $t \bar{t}$ production and decay parts of the process are connected via exchange of QCD partons, and NLO corrections to singly- and non-resonant topologies. Further technical aspects are discussed in the original publications [336, 25].







Fig. 23: Representative LO diagrams of doubly-resonant (upper line), singly-resonant (first diagram in lower line), and non-resonant type (last two diagrams in lower line).

### 10.3 NUMERICAL RESULTS

### 10.31 Input parameters and setup

In the following we compare $\mathrm{t} \overline{\mathrm{t}}$ and $\mathrm{WWb} \overline{\mathrm{b}}$ predictions for $\mathrm{W}^{+}\left(\rightarrow \nu_{\mathrm{e}} \mathrm{e}^{+}\right) \mathrm{W}^{-}\left(\rightarrow \mu^{-} \bar{\nu}_{\mu}\right) \mathrm{b} \overline{\mathrm{b}}$ production at the Tevatron ( $\mathrm{p} \overline{\mathrm{p}}$ collisions at 1.96 TeV ) and the LHC ( pp collisions at 7 and 14 TeV ). These results are based on the same input parameters and cuts as in Ref. [25]. In NLO (LO) QCD we employ MSTW2008NLO (LO) parton distributions [262] and describe the running of the strong coupling constant $\alpha_{\mathrm{S}}$ with two-loop (one-loop) accuracy, including five active flavours. Contributions induced by the strongly suppressed bottom-quark density are neglected. For the gauge-boson and top-quark masses we use $m_{\mathrm{t}}=172 \mathrm{GeV}, M_{\mathrm{W}}=80.399 \mathrm{GeV}$, and $M_{\mathrm{Z}}=91.1876 \mathrm{GeV}$. The masses of all other quarks, including b-quarks, are neglected. In view of the negligibly small Higgs-mass dependence we adopt the $M_{\mathrm{H}} \rightarrow \infty$ limit, i.e. we omit diagrams involving Higgs bosons. The electroweak couplings are derived

| Collider | $\sqrt{s}[\mathrm{TeV}]$ | approx. | $\sigma_{\mathrm{tt}}[\mathrm{fb}]$ | $\sigma_{\mathrm{WWb}}[\mathrm{fb}]$ | $\sigma_{\mathrm{tt}} / \sigma_{\mathrm{WWb}}-1$ | Ref. [25] |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Tevatron | 1.96 | LO | $44.691(8)_{-12.58}^{+19.81}$ | $44.310(3)_{-12.49}^{+19.68}$ | $+0.861(19) \%$ | $+0.8 \%$ |
|  |  | NLO | $42.16(3)_{-2.91}^{+0.00}$ | $41.75(5)_{-2.63}^{+0.00}$ | $+0.98(14) \%$ | $+0.9 \%$ |
| LHC | 7 | LO | $659.5(1)_{-173.1}^{+261.8}$ | $662.35(4)_{-174.1}^{+263.4}$ | $-0.431(16) \%$ | $-0.4 \%$ |
|  |  | NLO | $837(2)_{-87}^{+42}$ | $840(2)_{-87}^{+41}$ | $-0.41(31) \%$ | $-0.2 \%$ |
| LHC | 14 | LO | $3306.3(1)_{-763.6}^{+1086}$ | $3334.6(2)_{-771.2}^{+1098.5}$ | $-0.849(7) \%$ | --- |

Table 8: Integrated $\nu_{\mathrm{e}} \mathrm{e}^{+} \mu^{-} \bar{\nu}_{\mu} \mathrm{b} \overline{\mathrm{b}}$ cross section in narrow-with approximation $\left(\sigma_{\mathrm{t} \overline{\mathrm{t}}}\right)$ and including finite-top-width effects $\left(\sigma_{\mathrm{WWb}} \overline{\mathrm{b}}\right)$. The relative error of the narrow-width approximation (sixth column) is compared to the prediction of Ref. [25] (seventh column). Factor-two scale variations in $\sigma_{\mathrm{tt}}$ and $\sigma_{\mathrm{Wwb} \overline{\mathrm{b}}}$ are shown as sub- and super-scripts, while statistical errors are given in parenthesis.
from the Fermi constant $G_{\mu}=1.16637 \times 10^{-5} \mathrm{GeV}^{-2}$ in the $G_{\mu}$-scheme, where the sine of the mixing angle and the electromagnetic coupling read $s_{\mathrm{w}}^{2}=1-M_{\mathrm{W}}^{2} / M_{\mathrm{Z}}^{2}$ and $\alpha=\sqrt{2} G_{\mu} M_{\mathrm{W}}^{2} s_{\mathrm{w}}^{2} / \pi$. For consistency, we perform the LO and NLO calculations using the top-quark widths $\Gamma_{\mathrm{t}, \mathrm{LO}}=1.4655 \mathrm{GeV}$ and $\Gamma_{\mathrm{t}, \mathrm{NLO}}=1.3376 \mathrm{GeV}$ [340], respectively. Since the leptonic W-boson decay does not receive NLO QCD corrections we employ the NLO W-boson width $\Gamma_{\mathrm{W}}=2.0997 \mathrm{GeV}$ everywhere.

Final-state quarks and gluons with pseudo-rapidity $|\eta|<5$ are converted into infrared-safe jets using the anti- $k_{\mathrm{T}}$ algorithm [341]. For the Tevatron (LHC) we set the jet-algorithm parameter $R=0.4$ (0.5) and apply the transverse-momentum and pseudo-rapidity cuts $p_{\mathrm{T}, \mathrm{b}-\mathrm{jet}}>20(30) \mathrm{GeV},\left|\eta_{\mathrm{b}-\mathrm{jet}}\right|<2.5$. Moreover, we require a missing transverse momentum of $p_{\mathrm{T}, \mathrm{miss}}>25(20) \mathrm{GeV}$ and charged leptons with $p_{\mathrm{T}, l}>20 \mathrm{GeV}$ and $\left|\eta_{l}\right|<2.5$.

For the renormalisation and factorisation scales we adopt the central value $\mu=m_{\mathrm{t}}$ and study factor-two variations of $\mu=\mu_{\mathrm{ren}}=\mu_{\mathrm{fact}}$, i.e. we compare predictions at $\mu / m_{\mathrm{t}}=0.5,1,2$. The scale variations are applied also to $\Gamma_{\mathrm{t}, \mathrm{NLO}}$, but not to $\Gamma_{\mathrm{W}}$.

### 10.32 Integrated cross section

Results for the integrated $\nu_{\mathrm{e}} \mathrm{e}^{+} \mu^{-} \bar{\nu}_{\mu} \mathrm{b} \overline{\mathrm{b}}$ cross sections and scale uncertainties at the Tevatron and the LHC are reported in Table 8. While the $\sigma_{\text {Wwb币 }}$ results for Tevatron and LHC at 7 TeV correspond to those of Ref. [25] ${ }^{19}$, the ones for LHC at 14 TeV as well as all $\sigma_{\mathrm{t} \bar{\epsilon}}$ predictions are new. Comparing all $\mathrm{WWb} \overline{\mathrm{b}}$ and $t \bar{t}$ predictions we find that finite-top-width effects never exceed one percent, both in LO and NLO. The statistical precision of the calculations permits us to assess the error of the NWA, $\sigma_{\mathrm{t} \overline{\mathrm{t}}} / \sigma_{\mathrm{WWbb}}-1$, with an accuracy of $1-3$ permille. At the Tevatron, the NWA overestimates the WWb $\bar{b}$ cross section by an amount very close to $\Gamma_{\mathrm{t}} / m_{\mathrm{t}} \simeq 0.9 \%$, both in LO and NLO. The error of the NWA at the 7 (14) TeV LHC ranges between 4 and 8 permille. As shown in the last column of Table 8 these finite-width effects are in very good agreement with the results of the $\Gamma_{\mathrm{t}} \rightarrow 0$ extrapolation in Ref. [25]. Similar results can be found also in Ref. [23].

[^205]
### 10.33 Differential distributions

The small finite-width corrections to the integrated cross section demonstrate that-in presence of standard LHC and Tevatron cuts-the NWA provides a fairly accurate description of inclusive WWb̄ production. It is thus interesting to investigate to which extent this conclusion applies to the various phenomenologically important regions of the WWb $\overline{\mathrm{b}}$ phase space. To this end we have compared $\mathrm{t} \overline{\mathrm{t}}$ and WWbb predictions for a few differential observables that are relevant for top-pair production, either as signal or as background to Higgs production or new physics. Note that we refrain from selecting kinematic variables like the top-quark invariant mass or imposing cuts of type $M_{\mathrm{Wb}}>200 \mathrm{GeV}$, which would lead to obvious enhancements of non-resonant contributions.

In Figs. 2427 we present predictions for some invariant-mass and transverse-momentum distributions, restricting ourselves to the case of the 7 TeV LHC. For each observable we display $t \bar{t}$ (dashed curves) and $\mathrm{WWb} \overline{\mathrm{b}}$ (solid curves) results in LO (blue) and NLO (red) approximation. Absolute predictions (left plots) are complemented by the ratios $\left(\mathrm{d} \sigma_{\mathrm{LO}}-\mathrm{d} \sigma_{\mathrm{NLO}}\right) / \mathrm{d} \sigma_{\mathrm{NLO}}$ (upper right plots) and $\left(\mathrm{d} \sigma_{\mathrm{t} \bar{t}}-\mathrm{d} \sigma_{\mathrm{WWb} \overline{\mathrm{b}}}\right) / \mathrm{d} \sigma_{\mathrm{WWb}}$ (lower right plots), which indicate the relative error of LO and narrow-width approximations w.r.t. the best predictions, i.e. NLO and WWb $\overline{\mathrm{b}}$.


Fig. 24: Distribution in the transverse momentum of the harder b-jet at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb $\overline{\mathrm{b}}$, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrow-width (lower-right) approximations w.r.t. NLO and WWb̄ predictions, respectively.

The transverse-momentum distribution of the harder b-jet is shown in Fig. 24 In the range below 200 GeV , which contains the bulk of the cross section, the NLO and finite-width corrections behave similarly as for the integrated cross section: LO predictions deviate from NLO ones by about $-20 \%$, and the error of the NWA ranges between +1 and $-4 \%$. Finite-width effects tend to increase with $p_{\mathrm{T}}$ and reach the $10 \%$ level around 300 GeV . Within the entire $p_{\mathrm{T}}$ range the LO/NLO ratios resulting from the $t \bar{t}$ and WWbb̄ calculations are almost equal. Equivalently, we find the same $\mathrm{d} \sigma_{\mathrm{tt}} / \mathrm{d} \sigma_{\mathrm{WWbb}}$ ratios in LO and NLO.


Fig. 25: Distribution in the transverse momentum of the b̄ di-jet system at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb百, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrow-width (lower-right) approximations w.r.t. NLO and WWb̄ predictions, respectively.

In Fig. 25 we show the transverse-momentum distribution of the $b \bar{b}$ di-jet system. This kinematic variable plays an important role in boosted-Higgs searches with a large t $\bar{t}$ background. In particular, the strategy proposed in Ref. [342] to extract a pp $\rightarrow \mathrm{H}(\rightarrow \mathrm{b} \overline{\mathrm{b}}) \mathrm{W}$ signal at the LHC is based on the selection of boosted $\mathrm{H} \rightarrow \mathrm{b} \overline{\mathrm{b}}$ candidates with $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}}>200 \mathrm{GeV}$, which permits to reduce $\mathrm{t} \overline{\mathrm{t}}$ contamination (and other backgrounds) in a very efficient way. As can be seen from Fig. 25, the suppression of $t \bar{t}$ production is indeed particularly strong at $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}} \gtrsim 150 \mathrm{GeV}$. This is due to kinematic constraints that characterise the LO and narrow-width approximations: in order to acquire $p_{\mathrm{T}, \mathrm{b}}>\left(m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2}\right) /\left(2 m_{\mathrm{t}}\right) \simeq 65 \mathrm{GeV}$ b-quarks need to be boosted via the $p_{\mathrm{T}}$ of their parent (anti)top quarks, and the fact that top and antitop quarks have opposite transverse momenta (at LO) makes it difficult to generate a b $\bar{b}$ system with high $p_{\mathrm{T}}$. The NLO and finite-width corrections undergo less stringent kinematic restrictions, resulting into a significant enhancement of $W W b \overline{\mathrm{~b}}$ events at large $p_{\mathrm{T}, \mathrm{b}}$. This is clearly reflected in the differences between the various curves in the left plot of Fig. 25. The most pronounced effect comes from the NLO corrections, where the $t \bar{t}$ system can acquire large transverse momentum by recoiling against extra jet radiation. As indicated by the right-upper plot, the NLO correction represents $50-80 \%$ of the cross section at high $p_{\mathrm{T}}$, corresponding to a huge $K$-factor of $2-5$. Finite-width effects (lower-right plot) lead to a further significant, although less dramatic, enhancement; for example, non-resonant topologies can lead to direct b $\overline{\mathrm{b}}$ production via high- $p_{\mathrm{T}}$ gluons that recoil against $\mathrm{W}^{+} \mathrm{W}^{-}$pairs. For $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}}>200 \mathrm{GeV}$, we find that $20-40 \%$ of the LO WWbb cross section is due to finite-width contributions, while this fraction decreases to $7-15 \%$ at NLO. This reduction is related to the dominance of the jet-emission contribution, which we expect to be rather well described by the NWA. On the other hand, an optimal suppression of the $t \bar{t}$ background will require a very tight jet-veto [342], and in this case we expect finite-width corrections to the NLO t̄ predictions to be as large as in LO.

The distribution in the missing transverse momentum, i.e. the vector sum of the $\nu_{e}$ and $\bar{\nu}_{\mu}$ trans-


Fig. 26: Distribution in the missing transverse momentum at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb $\overline{\mathrm{b}}$, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrowwidth (lower-right) approximations w.r.t. NLO and WWb̄̄ predictions, respectively.
verse momenta, is displayed in Fig. 26. This distribution is relevant for new-physics searches based on missing transverse energy plus jets and leptons. Its tail features a qualitatively similar behaviour as in the case of $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}}$, due to analogous kinematic constraints. However, in the case of $p_{\mathrm{T}, \mathrm{miss}}$ the corrections are less pronounced: the NLO correction does not exceed $40-50 \%$ of the full prediction, and finite-width contributions stay below roughly $10 \%$.

Figure 27 displays the distribution in the invariant mass of the positron and a b-jet, i.e. the visible products of a top-quark decay. More precisely, assuming that the charge of the b-jet is not known, the $\mathrm{e}^{+} \mathrm{b}$ pair is built by selecting the b-jet that yields the smallest invariant mass ${ }^{20}$ In narrow-width and LO approximation this kinematic quantity is characterised by a sharp upper bound, $M_{\mathrm{e}^{+} \mathrm{b}}^{2}<m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2} \simeq$ $(152 \mathrm{GeV})^{2}$, which renders it very sensitive to the top-quark mass. The value of $m_{\mathrm{t}}$ can be extracted with high precision using, for instance, the invariant-mass distribution of a positron and a $J / \psi$ from a $B$ meson decay [343, 338], an observable that is closely related to $M_{\mathrm{e}^{+} \mathrm{b}}$. In the region below the kinematic bound, the NLO corrections to $M_{\mathrm{e}^{+} \mathrm{b}}$ vary between $5-30 \%$, and the impact of the NLO shape distortion on a precision $m_{\mathrm{t}}$-measurement is certainly significant. For $M_{\mathrm{e}^{+} \mathrm{b}}<150 \mathrm{GeV}$, the NWA agrees with the WWb $\bar{b}$ predictions at the $1 \%$ level or better. In contrast, in the vicinity of the kinematic bound the impact of finite-width (and NLO) corrections becomes clearly more important, giving rise to a tail that extends above $M_{\mathrm{e}^{+} \mathrm{b}}^{2}=m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2}$. The resulting contribution to the total cross section is fairly small, but the impact of such finite-width effects on the top-mass measurement might be non-negligible, given the high $m_{\mathrm{t}}$-sensitivity of the $M_{\mathrm{e}^{+} \mathrm{b}}^{2} \simeq m_{\mathrm{t}}^{2}-M_{\mathrm{W}}^{2}$ region.

[^206]

Fig. 27: Distribution in the invariant mass of the positron-b-jet system (as defined in the text) at the 7 TeV LHC: LO (blue) and NLO (red) predictions in narrow-width approximation ( $\mathrm{t} \overline{\mathrm{t}}$, dashed) and including finite-top-width effects (WWb $\bar{b}$, solid). Plotted are absolute predictions (left) and relative deviations of LO (upper-right) and narrow-width (lower-right) approximations w.r.t. NLO and WWb $\bar{b}$ predictions, respectively.

### 10.4 CONCLUSIONS

Based on recent NLO QCD calculations, we have presented a systematic comparison of top-pair production and decay in narrow-top-width approximation, $\mathrm{pp} \rightarrow \mathrm{t} \overline{\mathrm{t}} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$, against the complete $\mathrm{pp} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$ process, which involves finite-top-width effects of non-resonant and off-shell type.

At the Tevatron and the LHC ( 7 and 14 TeV ), finite-top-width contributions to the integrated cross section (in the di-lepton channel) turn out not to exceed one percent. This confirms previous estimates based on the $\Gamma_{\mathrm{t}} \rightarrow 0$ extrapolation of $\mathrm{pp} \rightarrow \mathrm{WWb} \overline{\mathrm{b}}$ predictions. At the 7 TeV LHC, we also investigated differential observables that are relevant either for top-pair production as a signal or as a background in Higgs or new-physics searches. In the case of the b-jet transverse momentum and $p_{\mathrm{T}, \mathrm{miss}}$ distributions, finite-width effects remain very small over a large kinematic range and reach the $10 \%$ level only around 300 GeV . In contrast, the $p_{\mathrm{T}}$-distribution of the b $\overline{\mathrm{b}}$ di-jet system receives $\Gamma_{\mathrm{t}}$-corrections beyond 20-30\% for $p_{\mathrm{T}, \mathrm{b} \overline{\mathrm{b}}} \gtrsim 200 \mathrm{GeV}$, a kinematic region that plays an important role in $\mathrm{pp} \rightarrow \mathrm{H}(\rightarrow \mathrm{b} \overline{\mathrm{b}}) \mathrm{W}$ searches based on boosted $\mathrm{H} \rightarrow \mathrm{b} \overline{\mathrm{b}}$ candidates. For the lepton-b-jet invariant-mass distribution-an observable that provides high sensitivity to the top-quark mass-finite-width corrections do not exceed one percent in the range that contains the bulk of the cross section, but become more sizable in the region of highest $m_{\mathrm{t}}$-sensitivity. This motivates more detailed studies of finite-width effects in the context of high-precision $m_{\mathrm{t}}$-measurements at the LHC. The results of this investigation of finite-width effects in t̄̄ production give also useful insights into possible limitations of treating associated top-pair production processes in the narrow-width approximation, since NLO calculations for $\mathrm{pp} \rightarrow \mathrm{WWb} \mathrm{\bar{b}}$ and similar reactions will not be available too soon.

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## 11. Strong and Smooth Ordering in Antenna Showers ${ }^{21}$


#### Abstract

We comment on strong and smooth ordering in antenna showers, and extend the definition of smooth ordering to include the case of $g \rightarrow q \bar{q}$ splittings. We define three observables in hadronic $Z$ decays that can be used to probe the subleading properties of shower models.


### 11.1 INTRODUCTION

Traditional parton showers are based on collinear factorization, and the shower evolution proceeds via $1 \rightarrow 2$ branchings, on which additional constraints have to be imposed to ensure momentum conservation and QCD coherence (see [344]). Antenna showers are instead based on momentum-conserving and intrinsically coherent $2 \rightarrow 3$ branchings, as pioneered by Ariadne [345, 346]. This note concerns the antenna shower implementation in the Vincia code [347], a plug-in to Pythia 8 [348], though we emphasize that the notion of smooth ordering could be applied to other shower types as well.

In leading-logarithmic (LL) antenna showers, the fundamental step is a Lorentz-invariant $2 \rightarrow 3$ branching process by which two on-shell "parent" partons are replaced by three on-shell "daughter" partons. This $2 \rightarrow 3$ process makes use of three ingredients [349]:

1. An antenna function that captures the leading tree-level singularities of QCD matrix elements.
2. An antenna phase space - an exact, momentum-conserving and Lorentz-invariant factorization of the pre- and post-branching phase spaces.
3. A kinematics map, specifying how the global orientation of the post-branching momenta are related to the pre-branching ones.
Antenna showers come in two varieties: global and sector. The two kinds differ in how the collinear singularities of gluons are partitioned among neighboring antennae, see [350, 351]. Here, we shall only be concerned with the global type [345, 352, 347, 349], in which the gluon-collinear singularity is partitioned such that two neigbouring antennae each contain "half" of it; their sum reproduces the full singularity.

If each antenna in a global shower is allowed to emit in its full phase space, the resulting shower evolution amounts to an incoherent addition of independently radiating dipoles. This tends to overcount regions in which several dipole terms contribute at the same level, i.e., in regions where dipole-dipole interference effects (or, equivalently, multipole effects) are important [353, 351]. The situation is analogous to, though less severe than, the case of traditional parton showers with virtuality-ordering [354], which represent an incoherent addition of independent monopoles. In parton/monopole showers, multiparton interference effects for soft radiation can be taken into account by the requirement of angular ordering [355], while in dipole/antenna showers, typically a measure of transverse momentum is used, such as

$$
\begin{equation*}
p_{\perp A}^{2}=\frac{s_{i j} s_{j k}}{s_{I K}} \tag{80}
\end{equation*}
$$

for a branching $I K \rightarrow i j k$, with $s_{a b} \equiv 2 p_{a} \cdot p_{b}=\left(p_{a}+p_{b}\right)^{2}$ for massless partons. Some alternative possibilities are compared in [349].

[^207]
### 11.2 STRONG AND SMOOTH ORDERING

In a strongly-ordered shower, each consecutive branching is required to occur at a lower scale in the evolution variable than that of the previous one: $Q_{n+1}<Q_{n}$. This can be represented as a step function in the evolution variable, multiplying the branching kernels. In a smoothly-ordered shower [349], the step function is replaced by a smooth dampening factor designed to leave the soft and collinear limits unchanged while suppressing radiation at scales above $\sim Q_{n}$. Specifically, for evolution in $p_{\perp}$, we replace the strong-ordering condition as follows,

$$
\begin{equation*}
\Theta\left(\hat{p}_{\perp}-p_{\perp}\right) P_{L L} \rightarrow P_{i m p} P_{L L} \equiv \frac{\hat{p}_{\perp}^{2}}{\hat{p}_{\perp}^{2}+p_{\perp}^{2}} P_{L L} \tag{81}
\end{equation*}
$$

where $\hat{p}_{\perp}$ characterizes the scale of the previous branching ${ }^{22}, p_{\perp}$ is the scale of the emission under consideration, and $P_{L L}$ is an ordinary LL shower kernel, which in our case is represented by a gluonemission antenna function. (We return to the case of $g \rightarrow q \bar{q}$ below.)

Thus, for $p_{\perp} \ll \hat{p}_{\perp}$ (the strongly-ordered limit) the smooth-ordering factor $P_{\text {imp }}$ tends to unity, while for $p_{\perp} \sim \hat{p}_{\perp}$ (the ordering threshold) it tends to $1 / 2$, and finally for $p_{\perp} \gg \hat{p}_{\perp}$ (highly unordered), it tends to zero $\propto \hat{p}_{\perp}^{2} / p_{\perp}^{2}$. Note that, since $P_{L L}$ is likewise $\propto 1 / p_{\perp}^{2}$, the net effect of the suppression factor is to modify the behavior of the splitting kernel from $1 / p_{\perp}^{2}$ in the strongly-ordered limits to $1 / p_{\perp}^{4}$ for highly unordered branchings, similar to what has been studied for initial-state parton showers in [356]; above the strong-ordering threshold, the branching probability is explicitly suppressed beyond LL.

For a rigourous interpretation of the $P_{\text {imp }}$ factor one would have to analyze the $2 \rightarrow 4$ antennae [79] and check that the combination of two $2 \rightarrow 3$ antennae times this factor does indeed reproduce subleading aspects of the full $2 \rightarrow 4$ function. In the absence of such a study, one may still physically interpret its purpose in the following way: the LL antenna functions are derived assuming the outgoing partons/jets to be massless. This is a good approximation if the virtuality that they can acquire (through further showering) is restricted by the strong-ordering threshold. When allowing unordered branchings, however, the corresponding Feynman diagrams contain highly off-shell propagators, which the $P_{\text {imp }}$ factor attempts to mimic by introducing an "effective mass" in the denominator of eq. 81.

For gluon emissions, it was shown in [349] that the smooth-ordering condition does lead to a systematic improvement in the shower. Since it simultaneously guarantees a complete phase-space coverage (contrary to the case for strong ordering [357, 349]), it is the default option in Vincia.

Antenna showers including $g \rightarrow q \bar{q}$ splittings were studied in [358], in which evolution in $m_{q \bar{q}}^{2}$ was introduced for such branchings. This is based on the observation [359] that the scale controlling the divergences of $g \rightarrow q \bar{q}$ splittings is the invariant mass of the pair, not its $p_{\perp}$. By analogy with the physical interpretation given to the $P_{\text {imp }}$ factor for gluon emissions above, it therefore seems well-motivated to study a "generalized" $P_{\text {imp }}$ factor where each scale depends on whether we are dealing with a gluon or a quark:

$$
\begin{equation*}
P_{i m p}=\frac{\hat{Q}_{E}^{2}}{\hat{Q}_{E}^{2}+Q_{E}^{2}}, \tag{82}
\end{equation*}
$$

where $Q_{E}$ is the evolution variable: $p_{\perp}$ for gluons and invariant mass for quark-antiquark pairs.
We can assess the improvement that this produces in the shower by plotting the ratio of the shower approximation vs. the LO matrix element for $Z \rightarrow q \bar{q}^{\prime} q^{\prime} \bar{q}$ and $Z \rightarrow q \bar{q}^{\prime} q^{\prime} g \bar{q}$. This is shown in fig. 28, where the histograms represent the distribution of $\log _{10}(\mathrm{PS} / \mathrm{ME})$ in a flat phase-space scan, normalized to unity (i.e., the same type of distributions that were shown in [349, 358, 351]). Points to the left of zero are undercounted by the shower approximation, while points to the right are overcounted. Although the agreement is by no means perfect, we do observe a slight improvement in the shower approximation

[^208]

Fig. 28: Comparison between generalized $\tilde{P}_{i m p}$ and "old" $P_{i m p}$ factor in the global shower approximations to LO matrix elements, for processes involving a $g \rightarrow q \bar{q}$ splitting. Left: $Z \rightarrow q \bar{q}^{\prime} q^{\prime} \bar{q}$. Right: $Z \rightarrow q \bar{q}^{\prime} q^{\prime} q \bar{q}$. In both cases, GKS matching to the LO matrix element for the preceding multiplicity ( $Z \rightarrow 3$ and $Z \rightarrow 4$, respectively) has been included, and the Ariadne factor was applied to $g \rightarrow q \bar{q}$ splittings.
when the $P_{i m p}$ factor is defined in terms of $Q_{E}$ (solid black histogram), as compared to the definition used previously (dashed histogram). Note that we used the so-called Ariadne factor in the shower approximation for all cases, see [358], and that the distributions were made including GKS matching to the preceding multiplicities [349].

### 11.3 SENSITIVE OBSERVABLES IN HADRONIC Z DECAYS

The properties of shower and matrix-element matching algorithms are coming under increasing scrutiny, not least due to the desire of achieving reliable descriptions of jet production and jet properties, such as jet substructure, for signal and background estimates at the LHC.

For final-state radiation, i.e., jet broadening and jet splitting, hadronic $Z$ decays are the main reference, with a large set of events shapes and jet resolutions/rates being used to constrain and tune shower algorithms (see, e.g., [360, 344]). However, in the logarithmically dominated regions, these observables are typically dominated by leading logs, and are well described by all coherent and reasonably well-tuned shower algorithms on the market. In order to probe the subleading properties in a more dedicated way, we have found the following three simple observables useful, each designed to isolate a specific aspect.

We consider hadronic $Z$ events (photon ISR is switched off, and matching beyond 3 jets is switched off for the strongly-ordered showers) and use the $k_{T}$ clustering algorithm [361] to cluster all events back to two jets. The $3 \rightarrow 2$ clustering scale is denoted $y_{23}=k_{T 3}^{2} / m_{Z}^{2}$, and so on for higher jet numbers. We require all $y_{i j}$ entering in the observables below to be greater than 0.005 , to remove contamination from $B$ decays and lower scales. Since the original topology contains two jets, we also keep track of which "side" each clustering happens on. Strong ordering corresponds to $y_{23} \gg y_{34} \gg \ldots$, while events with, e.g., $y_{34} \sim y_{23}$ should be more sensitive to the ordering condition and to the effective $1 \rightarrow 3$ spliting kernels.

The first observable is thus simply the ratio $y_{34} / y_{23}$, in events where the $4 \rightarrow 3$ and $3 \rightarrow 2$ clusterings happen in the same jet. This distribution is illustrated in the left-hand pane of fig. 29, with logarithmic axes. Vertical error bars indicate the expected $1 \sigma$ statistical error with 400 k hadronic $Z$ decays. Since the $k_{T}$ algorithm allows for unordered clustering scales, the distribution extends beyond $\xi_{24}=\ln \left(y_{34} / y_{24}\right)=0$. Default Pythia (thick solid line) is compared to three different Vincia settings: smooth (thin solid) and strong (dashed) ordering in $p_{\perp}$ and strong ordering in dipole virtuality, $m_{D}$ (dotted). Note here that ordering in the variables $p_{\perp}$ or $m_{D}$ does not directly imply ordering in $k_{T}$.


Fig. 29: Left: $\xi_{24}=\ln \left(y_{34} / y_{23}\right)$ in "same-side" 4-jet events. Right: Ratio of jet masses, $m_{L}^{2} / m_{H}^{2}$, in "compressed" 4-jet events. Error bars indicate expected $1 \sigma$ statistical errors with 400 k hadronic $Z$ decays.

The fact that the $P_{\text {imp }}$ factor also suppresses branchings slightly below the strong-ordering threshold is manifest in the thin solid line lying below the other ones in the region just below zero, which should be statistically significant with a sample size of $\sim 0.5 \mathrm{M}$ events. Note as well that these distributions become indistinguishable if one does not make the requirement of sameside clustering (not shown), presumably since opposite-side collinear splittings then dominate.

A related observable is shown in the right-hand pane of fig. 29. To force a "compressed" scale hierarchy, we impose the cut $y_{34}>0.5 y_{23}$, and plot the ratio $M_{L}^{2} / M_{H}^{2}$ of the masses of the jets at the end of the clustering. With four partons at LO, the light jet mass is zero if both the $4 \rightarrow 3$ and $3 \rightarrow 2$ clusterings happen in the same jet, while it is non-zero otherwise. Thus, the region close to zero isolates events with a $1 \rightarrow 3$ splitting occurring in one of the jets, while the region above $\sim 0.25$ is dominated by opposite-side $1 \rightarrow 2$ splittings. In Pythia and in mass-ordered Vincia, the peak at zero is stronger than in the $p_{\perp}$-ordered Vincia cases, while there is no difference between strong and smooth ordering in this variable. It thus serves as a useful complement to $\xi_{24}$.

Finally, in fig. 30, we consider 4-jet events in which the second and third jets (ordered in energy) are nearly collinear and back-to-back to the hardest jet. Specifically, we impose the cuts $\theta_{12}>120^{\circ}$, $\theta_{13}>120^{\circ}$, and $\theta_{23}<30^{\circ}$. We then plot the angle of the fourth (softest) jet with respect to the hardest one. Again the strong and smooth ordering options are indistinguishable, but interesting differences with respect to both Pythia and mass-ordered Vincia are visible. Mass-ordering tends to produce a broader distribution, with more radiation at right angles to the hardest jet (consistent with mass-ordering prioritizing wide-angle emissions over collinear ones), and the $p_{\perp}$-ordered Vincia showers exhibit a stronger collinear peak than the Pythia one. A similar observable was proposed in [362].

We conclude that, if all three observables could be measured with an accuracy of $\sim 5-10 \%$ or better, a useful and multi-dimensional constraint on the subleading shower aspects would be obtained, including sensitivity both to the type and shape of the ordering condition, and to the form of the effective $1 \rightarrow 3$ probabilities produced by the shower. We emphasize that we have here restricted our attention to shower models that are virtually indistinguishable on all other observables we have considered.

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Fig. 30: Angle between the hardest $\left(1^{\text {st }}\right)$ and softest $\left(4^{\text {th }}\right)$ jets in "collinear" 4 -jet events. Error bars indicate expected $1 \sigma$ statistical errors with 400 k hadronic $Z$ decays.
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## 12. PERTURBATIVE UNCERTAINTIES AND RESUMMATION FOR EXCLUSIVE JET CROSS SECTIONS ${ }^{23}$

### 12.1 Introduction

In this writeup we discuss predictions for exclusive jet cross sections, which have a particular number of jets in the final state. There are several motivations for analyzing events by dividing the data into exclusive jet bins, in particular when the relevant backgrounds strongly depend on the number of jets, or when the sensitivity can be increased by optimizing the analysis for the individual jet bins. As our primary example we will consider the Higgs analysis in the $H \rightarrow W W$ channel, which is performed separately in exclusive 0 -jet, 1 -jet, and 2 -jet bins [363, 364, 365]. Other examples are vector-boson fusion analyses, which are typically performed in the exclusive 2-jet channel, boosted $H \rightarrow b \bar{b}$ analyses that include a veto on additional jets, as well as $H \rightarrow \tau \tau$ and $H \rightarrow \gamma \gamma$ which benefit from improved sensitivity when the Higgs recoils against a jet. The importance of the Higgs +1 jet channel in $H \rightarrow \tau \tau$ and $H \rightarrow W W^{*}$ was demonstrated explicitly in Refs. [366, 367]. Another motivation for studying exclusive jet bins are the $W+$ jets channels, which are important backgrounds for new physics searches. We will use the notation $\sigma_{N}$ for an exclusive $N$-jet cross section (with exactly $N$ jets), and the notation $\sigma_{\geq N}$ for an inclusive $N$-jet cross section (with $N$ or more jets).

To explore the implications of the jet bin restrictions, consider a simple example where we divide the total cross section, $\sigma_{\text {total }}$, into an exclusive 0 -jet bin, $\sigma_{0}\left(p^{\mathrm{cut}}\right)$, and the remaining inclusive $(\geq 1)$-jet bin, $\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right)$,

$$
\begin{equation*}
\sigma_{\mathrm{total}}=\int_{0}^{p^{\mathrm{cut}}} d p \frac{d \sigma}{d p}+\int_{p^{\mathrm{cut}}} d p \frac{d \sigma}{d p} \equiv \sigma_{0}\left(p^{\mathrm{cut}}\right)+\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right) . \tag{83}
\end{equation*}
$$

Here $p$ denotes the kinematic variable which is used to divide up the cross section into jet bins. A typical choice is $p \equiv p_{T}^{\text {jet }}$, defined by the largest $p_{T}$ of any jet in the event, such that $\sigma_{0}\left(p_{T}^{\text {cut }}\right)$ only contains events with jets having $p_{T} \leq p_{T}^{\mathrm{cut}}$, and $\sigma_{\geq 1}\left(p_{T}^{\mathrm{cut}}\right)$ contains events with at least one jet with $p_{T} \geq p_{T}^{\text {cut }}$. By defining $\sigma_{0}\left(p_{T}^{\text {cut }}\right)$ and $\sigma_{\geq 1}\left(p_{T}^{\text {cut }}\right)$ one has divided up initial-state radiation from the

[^209]colliding hard partons and soft radiation in the event. This restriction on additional emissions changes the coefficients appearing in the $\alpha_{s}$ expansion and leads to the appearance of double and single logarithms of the form $\alpha_{s} \ln ^{2}\left(p^{\text {cut }} / Q\right)$ and $\alpha_{s} \ln \left(p^{\text {cut }} / Q\right)$ (with higher powers $\alpha_{s}^{n} \ln ^{m \leq 2 n}\left(p^{\text {cut }} / Q\right)$ appearing at higher orders in perturbation theory). Here $Q$ is the hard scale of the process, such as $Q=m_{H}$ for Higgs production, and most often we have $p^{\text {cut }} \ll Q$. These changes to the perturbation series can modify the convergence of fixed-order results and make it prudent to consider resummed cross section predictions that include an all-orders resummation of the large logarithms. For $N$ jets the analog of Eq. 833) is $\sigma_{\geq N}=\sigma_{N}\left(p_{N+1}^{\mathrm{cut}}\right)+\sigma_{\geq N+1}\left(p_{N+1}^{\mathrm{cut}}\right)$ and the same discussion applies regarding the large logarithms of $p_{N}^{\text {cut }}$ that are not present in $\sigma_{\geq N}$, but are present in each of $\sigma_{N}$ and $\sigma_{\geq N+1}$.

The definition of $\sigma_{0}\left(p^{\mathrm{cut}}\right)$ may include dependence on rapidity and on the grouping of particles. For a jet-based variable like $p_{T}^{\text {jet }}$ the former is induced by only considering jets within the rapidity range $\left|\eta^{\text {jet }}\right| \leq \eta^{\text {cut }}$, and the latter enters through the choice of jet algorithm. These dependencies make theoretical predictions more difficult. In Higgs production via gluon fusion the cross section is known to next-to-next-to-leading order (NNLO) [208, 368, 207, 209, 210, 211, 369, 370], and NNLO results including full kinematic information are available through FeHiP [214, 371] and HNNLO [90, 216] (as well as by combining the total NNLO cross section with MCFM [157, 372] for some distributions). When the measurements are performed in exclusive jet bins, the perturbative uncertainties in the theoretical predictions must also be evaluated separately for each individual jet bin [373]. When combining channels with different jet multiplicities, the correlations between the theoretical uncertainties can be significant and must be taken into account [26]. The perturbative predictions can be made more precise by including a resummation of large $p^{\text {cut }}$ dependent logarithms on top of the fixed-order predictions. At the leading logarithmic level this can be achieved with standard parton shower Monte Carlo programs, regardless of the precise definition of $p^{\mathrm{cut}}$. So far a next-to-next-to-leading logarithmic (NNLL) resummed result for a jet-veto variable only exists for beam thrust [374], $\mathcal{T}_{\mathrm{cm}}$, which is a rapidity weighted $E_{T}$-like inclusive variable. The definitions of the jet-veto variables we will use are

$$
\begin{equation*}
p_{T}^{\text {jet }}=\left|\sum_{k \in \mathrm{jet}} \vec{p}_{T k}\right|, \quad \quad \mathcal{T}_{\mathrm{cm}}=\sum_{k}\left|\vec{p}_{T k}\right| e^{-\left|\eta_{k}\right|}=\sum_{k}\left(E_{k}-\left|p_{k}^{z}\right|\right) . \tag{84}
\end{equation*}
$$

For $p_{T}^{\text {jet }}$ our jets are defined using anti- $k_{T}$ [341] with $R=0.5$, and we consider jets that satisfy a rapidity cut $|\eta| \leq \eta^{\text {cut }}$. For $\mathcal{T}_{\text {cm }}$ the sum is over all objects in the final state except the Higgs decay products, and can in principle be considered over particles, topo-clusters, or jets with a small $R$ parameter. In all our results we consistently use MSTW2008 NNLO PDFs [262].

In this writeup we will explore fixed NNLO and resummed NNLL+NNLO predictions for $H+$ 0 -jet cross sections and compare various methods for evaluating the uncertainty as a function of cuts on $p_{T}^{\text {jet }}$ and $\mathcal{T}_{\mathrm{cm}}$. The three methods we will discuss for evaluating the uncertainties in exclusive jet cross sections are
A) "Direct Exclusive Scale Variation". Here the uncertainties are evaluated by directly varying the renormalization and factorization scales in the fixed-order predictions for each exclusive jet cross section $\sigma_{N}$. This implies that the uncertainties are $100 \%$ correlated for different $N$ s.
B) "Combined Inclusive Scale Variation", as proposed in Ref. [26] and utilized in Refs. [363, 364 365]. Here, the perturbative uncertainties in the inclusive $N$-jet cross sections, $\sigma_{\geq N}$, are treated as the primary uncertainties that can be evaluated by scale variations in fixed-order perturbation theory. These uncertainties are treated as uncorrelated for different $N$. The exclusive $N$-jet cross sections are obtained using $\sigma_{N}=\sigma_{\geq N}-\sigma_{\geq N+1}$. The uncertainties and correlations follow from standard error propagation, including the appropriate anticorrelations between $\sigma_{N}$ and $\sigma_{N \pm 1}$ related to the division into jet bins.
C) "Uncertainties from Resummation." Resummed calculations for exclusive jet cross sections can provide uncertainty estimates that allow one to simultaneously include both types of correlated
and anticorrelated uncertainties as in methods A and B. The magnitude of the uncertainties may also be reduced from the resummation of large logarithms.
In all three methods, adding the exclusive jet cross sections yields the expected scale variation in the total cross section. Method B avoids a potential underestimate of the uncertainties in individual jet bins due to strong cancellations that can potentially take place in method A. Method B produces realistic perturbative uncertainties for exclusive jet cross sections when using fixed-order predictions for various processes, since it accounts for the presence of large logarithms at higher orders caused by the jet binning. In Method C one utilizes higher-order resummed predictions for the exclusive jet cross sections, which allow one to obtain improved central values and further refined uncertainty estimates.

The basic structure of the large logarithms in the perturbative series is discussed in Sec. 12.2. In Sec. 12.3 we discuss and compare the above three methods to determine the perturbative uncertainties. The work discussed here regarding methods A, B, and C builds on work done in Refs. [375, 26], was initiated at Les Houches, and has also been incorporated in the second Higgs Yellow Book report [376] (Secs. 5.2 and 5.5.) We also review recent work by others that can be found in [376](Sec. 5.3).

Note that here we are only discussing the theoretical uncertainties due to unknown higher-order perturbative corrections, which are commonly estimated using scale variation. Parametric uncertainties, such as PDF choices and $\alpha_{s}\left(m_{Z}\right)$ uncertainties, must be treated appropriately as common sources for all investigated channels.

### 12.2 Theoretical Motivation

### 12.21 Structure of the Perturbative Series

We begin by discussing the structure of the large logarithms in exclusive jet cross sections. For Higgs production from gluon fusion with $p_{T}^{\text {jet }} \leq p_{T}^{\text {cut }}$ the leading double logarithms appearing at $\mathcal{O}\left(\alpha_{s}\right)$ are

$$
\begin{equation*}
\sigma_{0}\left(p_{T}^{\mathrm{cut}}\right)=\sigma_{B}\left(1-\frac{3 \alpha_{s}}{\pi} 2 \ln ^{2} \frac{p_{T}^{\mathrm{cut}}}{m_{H}}+\cdots\right), \tag{85}
\end{equation*}
$$

where $\sigma_{B}$ is the Born (tree-level) cross section.
The total cross section only depends on the hard scale $Q=m_{H}$, which means by choosing the factorization and renormalization scales $\mu_{f} \simeq \mu_{r} \simeq m_{H}$, the fixed-order expansion does not contain large logarithms and has the structure

$$
\begin{equation*}
\sigma_{\text {total }} \simeq \sigma_{B}\left[1+\alpha_{s}+\alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] . \tag{86}
\end{equation*}
$$

Our expressions for perturbative series such as this one are schematic, showing the scaling of the terms without the coefficient functions. The convolution with the parton distribution functions (PDFs) are also not displayed. For $g g \rightarrow H$, the coefficients of this series can be large, corresponding to the well-known large K factors. As usual, varying the scale in $\alpha_{s}(\mu)$ (and the PDFs) one obtains an estimate of the size of the missing higher-order terms in this series, which we denote by $\Delta_{\text {total }}$.

The inclusive 1 -jet cross section has the perturbative structure

$$
\begin{equation*}
\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right) \simeq \sigma_{B}\left[\alpha_{s}\left(L^{2}+L+1\right)+\alpha_{s}^{2}\left(L^{4}+L^{3}+L^{2}+L+1\right)+\mathcal{O}\left(\alpha_{s}^{3} L^{6}\right)\right], \tag{87}
\end{equation*}
$$

where the logarithms $L=\ln \left(p^{\text {cut }} / m_{H}\right)$. For $p^{\text {cut }} \ll m_{H}$ these logarithms can get large enough to overcome the $\alpha_{s}$ suppression. In the limit $\alpha_{s} L^{2} \simeq 1$, the fixed-order perturbative expansion breaks down and the logarithmic terms must be resummed to all orders in $\alpha_{s}$ to obtain a meaningful result. For typical experimental values of $p^{\text {cut }}$ fixed-order perturbation theory can still be considered, but the logarithms cause large corrections at each order and dominate the series.

The exclusive 0 -jet cross section is equal to the difference between Eqs. (86) and (87), and so has the schematic structure
$\sigma_{0}\left(p^{\mathrm{cut}}\right)=\sigma_{\text {total }}-\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right)$

$$
\begin{equation*}
\simeq \sigma_{B}\left\{\left[1+\alpha_{s}+\alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right]-\left[\alpha_{s}\left(L^{2}+L+1\right)+\alpha_{s}^{2}\left(L^{4}+L^{3}+L^{2}+L+1\right)+\mathcal{O}\left(\alpha_{s}^{3} L^{6}\right)\right]\right\} \tag{88}
\end{equation*}
$$

In this difference, the large positive corrections in $\sigma_{\text {total }}$ partly cancel against the large negative logarithmic corrections in $\sigma_{\geq 1}$. For example, at $\mathcal{O}\left(\alpha_{s}\right)$ there is a value of $L$ for which the $\alpha_{s}$ terms in Eq. (88) cancel exactly. At this $p^{\text {cut }}$ the NLO 0 -jet cross section has vanishing scale dependence and is equal to the LO cross section, $\sigma_{0}\left(p^{\mathrm{cut}}\right)=\sigma_{B}$. Due to this cancellation, a standard use of scale variation in $\sigma_{0}\left(p^{\mathrm{cut}}\right)$ does not actually probe the size of the large logarithms, and does not provide an estimate of $\Delta_{\text {cut }}$. This issue impacts the uncertainties in the experimentally relevant region for $p^{\text {cut }}$.

For example, for $g g \rightarrow H$ (with $\sqrt{s}=7 \mathrm{TeV}, m_{H}=165 \mathrm{GeV}, \mu_{f}=\mu_{r}=m_{H} / 2$ ), one finds [214, 371, 90, 216]

$$
\begin{align*}
\sigma_{\text {total }} & =(3.32 \mathrm{pb})\left[1+9.5 \alpha_{s}+35 \alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] \\
\sigma_{\geq 1}\left(p_{T}^{\mathrm{jet}} \geq 30 \mathrm{GeV},\left|\eta^{\mathrm{jet}}\right| \leq 3.0\right) & =(3.32 \mathrm{pb})\left[4.7 \alpha_{s}+26 \alpha_{s}^{2}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] \tag{89}
\end{align*}
$$

In $\sigma_{\text {total }}$ one can see the impact of the well-known large $K$ factors. (Using instead $\mu_{f}=\mu_{r}=m_{H}$ the $9.5 \alpha_{s}$ and $35 \alpha_{s}^{2}$ coefficients in $\sigma_{\text {total }}$ increase to $11 \alpha_{s}$ and $65 \alpha_{s}^{2}$.) In $\sigma \geq 1$, one can see the impact of the large logarithms on the perturbative series. Taking their difference to get $\sigma_{0}$, one observes a sizeable numerical cancellation between the two series at each order in $\alpha_{s}$.

### 12.22 Perturbative Series for the Event Fraction

Experimentally the desired quantity which incorporates the jet-veto cut is the exclusive 0-jet event fraction

$$
\begin{equation*}
f_{0}\left(p^{\mathrm{cut}}\right)=\frac{\sigma_{0}\left(p^{\mathrm{cut}}\right)}{\sigma_{\mathrm{total}}}=1-\frac{\sigma_{\geq 1}\left(p^{\mathrm{cut}}\right)}{\sigma_{\mathrm{total}}} . \tag{90}
\end{equation*}
$$

One option for treating $f_{0}\left(p^{\mathrm{cut}}\right)$ is to consider it as a derived quantity, given the basic observables $\left\{\sigma_{0}, \sigma_{\text {total }}\right\}$ or $\left\{\sigma_{\geq 1}, \sigma_{\text {total }}\right\}$. In this approach, which was utilized in Ref. [26] and Ref. [376](Secs. 5.2 and 5.5), one propagates the uncertainties from the $\sigma_{i} \mathrm{~s}$ to derive those for $f_{0}\left(p^{\mathrm{cut}}\right)$. This approach is natural from the perspective of utilizing log-resummed computations for $\sigma_{0}\left(p^{\mathrm{cut}}\right)$. In particular, it maintains the constraint that for large $p^{\text {cut }}$ we have monotonic convergence of $\sigma_{0} \rightarrow \sigma_{\text {total }}$ and $f_{0} \rightarrow 1$, a property that relies on a phase space cut reducing the cross section, but does not depend on perturbation theory.

When using fixed-order predictions for the various cross sections, an alternative to Eq. (90) considered in Ref. [376](Sec. 5.3) is to analyze the perturbation theory for $f_{0}\left(p^{\mathrm{cut}}\right)$ directly. In this case different schemes of organizing the perturbation series, by keeping or dropping various $\mathcal{O}\left(\alpha_{s}^{3}\right)$ terms, give a method to estimate the size of the higher-order perturbative corrections. Three such schemes were considered in Ref. [376](Sec. 5.3) (which we label here by schemes 1,2,3). It is convenient to define the perturbative corrections to the cross section by dividing each of them by the Born cross section $\sigma_{B}$, such that we can write

$$
\begin{align*}
\sigma_{\text {total }} & =\sigma_{B}\left[1+\hat{\sigma}_{\text {total }}^{(1)}+\hat{\sigma}_{\text {total }}^{(2)}+\mathcal{O}\left(\alpha_{s}^{3}\right)\right], \\
\sigma_{\geq 1}\left(p^{\text {cut }}\right) & =\sigma_{B}\left[\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\text {cut }}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\text {cut }}\right)+\mathcal{O}\left(\alpha_{s}^{3}\right)\right] . \tag{91}
\end{align*}
$$

With this notation the result of treating $f_{0}$ as a derived quantity is

$$
\begin{equation*}
\left[f_{0}\left(p^{\mathrm{cut}}\right)\right]^{(\text {scheme } 1)}=1-\frac{\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\mathrm{cut}}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\mathrm{cut}}\right)}{1+\hat{\sigma}_{\text {total }}^{(1)}+\hat{\sigma}_{\text {total }}^{(2)}}+\mathcal{O}\left(\alpha_{s}^{3}\right), \tag{92}
\end{equation*}
$$

while at the same order in perturbation theory we can also consider the following expressions for $f_{0}$ :

$$
\begin{align*}
& {\left[f_{0}\left(p^{\mathrm{cut}}\right)\right]^{\text {(scheme } 2)}=1-\frac{\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\mathrm{cut}}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\mathrm{cut}}\right)}{1+\hat{\sigma}_{\text {total }}^{(1)}}+\mathcal{O}\left(\alpha_{s}^{3}\right),} \\
& {\left[f_{0}\left(p^{\mathrm{cut}}\right)\right]^{(\text {scheme } 3)}=1-\left[\hat{\sigma}_{\geq 1}^{(1)}\left(p^{\mathrm{cut}}\right)+\hat{\sigma}_{\geq 1}^{(2)}\left(p^{\mathrm{cut}}\right)\right]+\hat{\sigma}_{\geq 1}^{(1)} \hat{\sigma}_{\text {total }}^{(1)}+\mathcal{O}\left(\alpha_{s}^{3}\right) .} \tag{93}
\end{align*}
$$

We will contrast using the expressions in Eq. (92) and Eq. (93) with various methods for analyzing the uncertainty in our discussion below.

### 12.3 Uncertainty Analysis for Exclusive Jet Bins

As described in Sec. 12.21, the phase space restriction defining $\sigma_{0}$ changes its perturbative structure compared to that of $\sigma_{\text {total }}$. In general this gives rise to an additional perturbative uncertainty due to missing higher-order terms depending on $p^{\text {cut }}$. We will call the associated jet-binning uncertainty $\Delta_{\text {cut }}$. This can be thought of as an uncertainty related to the presence of large logarithms of $p^{\text {cut }}$ at higher orders in perturbation theory. In Eq. (83) both $\sigma_{0}$ and $\sigma_{\geq 1}$ depend on the phase space cut, $p^{\text {cut }}$, and by construction this dependence cancels in $\sigma_{0}+\sigma_{\geq 1}$. Hence, the additional uncertainty $\Delta_{\text {cut }}$ induced by $p^{\text {cut }}$ must be $100 \%$ anticorrelated between $\sigma_{0}\left(p^{\text {cut }}\right)$ and $\sigma_{\geq 1}\left(p^{\text {cut }}\right)$, such that it cancels in their sum. For example, using a covariance matrix to model the uncertainties and correlations, the contribution of $\Delta_{\text {cut }}$ to the covariance matrix for $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ must be of the form

$$
C_{\mathrm{cut}}=\left(\begin{array}{cc}
\Delta_{\mathrm{cut}}^{2} & -\Delta_{\mathrm{cut}}^{2}  \tag{94}\\
-\Delta_{\mathrm{cut}}^{2} & \Delta_{\mathrm{cut}}^{2}
\end{array}\right) .
$$

The questions then are: (1) How can we estimate $\Delta_{\text {cut }}$ in a simple way, and (2) how is the perturbative uncertainty $\Delta_{\text {total }}$ of $\sigma_{\text {total }}$ related to the uncertainties of $\sigma_{0}$ and $\sigma_{\geq 1}$ ?

### 12.31 Perturbative Uncertainties for Method A

When using method A to estimate the perturbative uncertainties one simply uses a common scale variation to estimate the uncertainty $\Delta_{0}$ in $\sigma_{0}$ and the uncertainty $\Delta_{\geq 1}$ in $\sigma_{\geq 1}$. By doing so the uncertainties are $100 \%$ correlated, corresponding to a covariance matrix in method A for $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ given by

$$
C_{A}=\left(\begin{array}{cc}
\Delta_{0}^{2} & \Delta_{0} \Delta_{\geq 1}  \tag{95}\\
\Delta_{0} \Delta_{\geq 1} & \Delta_{\geq 1}^{2}
\end{array}\right)
$$

Here $\Delta_{\text {total }}=\Delta_{0}+\Delta_{\geq 1}$ is the scale uncertainty in $\sigma_{\text {total }}$. When instead of $\sigma_{0}$ we directly calculate the 0 -jet event fraction $f_{0}$ using Eq. (92) or one of the expressions in Eq. (93), we can again determine the method A uncertainty estimate by scale variation in $f_{0}$ (we will refer to these results as methods $A_{1}, A_{2}$, and $A_{3}$ respectively).

In this method $\Delta_{\text {cut }}$ is not included because, as explained below Eq. (88), varying the perturbative scale in $\Delta_{0}$ does not probe the presence of the higher order large logarithms depending on $p^{\text {cut }}$. This method can lead to an underestimate of the perturbative uncertainty in $\sigma_{0}$ (and hence $f_{0}$ ), since there is a region of $p^{\text {cut }}$ values where scale variation is no longer a reasonable estimate of higher order corrections because of the vanishing of the $\mu$ dependence.

### 12.32 Perturbative Uncertainties for Method B

Since the perturbative series for $\sigma_{\geq 1}$ in Eq. (87) is dominated by the large logarithms of $p^{\text {cut }}$, we can use its scale variation $\Delta_{\geq 1}$ to get an estimate for their size by taking $\Delta_{\text {cut }}=\Delta_{\geq 1}$ [26]. Since $\Delta_{\text {cut }}$ and $\Delta_{\text {total }}$ are by definition uncorrelated, by setting $\Delta_{\text {cut }}=\Delta_{\geq 1}$ we are effectively treating the perturbative
series for $\sigma_{\text {total }}$ and $\sigma_{\geq 1}$ as independent with uncorrelated perturbative uncertainties. That is, considering $\left\{\sigma_{\text {total }}, \sigma_{\geq 1}\right\}$, the covariance matrix is diagonal,

$$
\left(\begin{array}{cc}
\Delta_{\text {total }}^{2} & 0  \tag{96}\\
0 & \Delta_{\geq 1}^{2}
\end{array}\right)
$$

where $\Delta_{\text {total }}$ and $\Delta_{\geq 1}$ are evaluated by separate scale variations in the fixed-order predictions for $\sigma_{\text {total }}$ and $\sigma_{\geq 1}$. This is consistent, since for small $p^{\text {cut }}$ the two series have very different structures. In particular, there is no reason to believe that the same cancellations in $\sigma_{0}$ will persist at every order in perturbation theory at a given $p^{\text {cut }}$. It follows that the perturbative uncertainty in $\sigma_{0}=\sigma_{\text {total }}-\sigma_{\geq 1}$ is given by $\Delta_{\text {total }}^{2}+\Delta_{\geq 1}^{2}$, and the resulting covariance matrix for $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ in method B is

$$
C_{B}=\left(\begin{array}{cc}
\Delta_{\geq 1}^{2}+\Delta_{\text {total }}^{2} & -\Delta_{\geq 1}^{2}  \tag{97}\\
-\Delta_{\geq 1}^{2} & \Delta_{\geq 1}^{2}
\end{array}\right) .
$$

Note that all of $\Delta_{\text {total }}$ occurs in the uncertainty for $\sigma_{0}$. This is reasonable from the point of view that $\sigma_{0}$ starts at the same order in $\alpha_{s}$ as $\sigma_{\text {total }}$ and contains the same leading virtual corrections. The method B uncertainty for the event fraction $f_{0}$ follows most naturally by error propagation from the cross sections, treating it as a derived quantity.

The limit $\Delta_{\text {cut }}=\Delta_{\geq 1}$ that Eq. (97) is based on is of course an approximation. However, the preceding arguments show that it is a more reasonable starting point than method A , since the latter does not account for the additional $p^{\text {cut }}$ induced uncertainties.

The generalization of the above discussion to more jets and several jet bins is straightforward. For the $N$-jet bin we replace $\sigma_{\text {total }} \rightarrow \sigma_{\geq N}, \sigma_{0} \rightarrow \sigma_{N}$, and $\sigma_{\geq 1} \rightarrow \sigma_{\geq N+1}$. If the perturbative series for $\sigma_{\geq N}$ exhibits large $\alpha_{s}$ corrections due to its logarithmic series or otherwise, then the presence of a different series of large logarithms in $\sigma_{\geq N+1}$ will again lead to cancellations when we consider the difference $\sigma_{N}=\sigma_{\geq N}-\sigma_{\geq N+1}$. These two cross sections will have different series for their double logarithms since the number of active partons and their color structure differ. In this situation $\Delta_{\geq N+1}$ will again give a better estimate for the extra $\Delta_{\text {cut }}$ type uncertainty that arises from separating $\sigma_{\geq N}$ into $\sigma_{N}$ and $\sigma_{\geq N+1}$.

### 12.33 Perturbative Uncertainties for Method C

In method C we assess the perturbative uncertainties using resummed predictions for variables $p^{\text {cut }}$ that implement a jet veto, following Refs. [375, 26]. An advantage of using resummed predictions is that they contain perturbation theory scale parameters which allow for an evaluation of two components of the theory error, one which is $100 \%$ correlated with the total cross section (as in method A), and one related to the presence of the jet-bin cut which is anti-correlated between neighboring jet bins (as in method B).

The resummed $H+0$-jet cross section predictions of Ref. [375] follow from a factorization theorem for the 0 -jet cross section [374], $\sigma_{0}\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)=H \mathcal{I}_{g i} \mathcal{I}_{g j} \otimes S f_{i} f_{j}$, where $H$ contains hard virtual effects, the $\mathcal{I}_{\text {s }}$ and $S$ describe the veto-restricted collinear and soft radiation, and the $f$ s are standard parton distributions. Fixed-order perturbation theory is carried out at three scales, a hard scale $\mu_{H}^{2} \sim m_{H}^{2}$ in $H$, and beam and soft scales $\mu_{B}^{2} \sim m_{H} \mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$ and $\mu_{S}^{2} \sim\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)^{2}$ for $\mathcal{I}$ and $S$, and are then connected by NNLL renormalization group evolution that sums the jet-veto logarithms, which are encoded in ratios of these scales. The perturbative uncertainties can be assessed by considering two sources: i) an overall scale variation that simultaneously varies $\left\{\mu_{H}, \mu_{B}, \mu_{S}\right\}$ up and down by a factor of two which we denote by $\Delta_{H 0}$, and ii) individual variations of $\mu_{B}$ or $\mu_{S}$ that each hold the other two scales fixed [375], whose envelope we denote by the uncertainty $\Delta_{S B}$. Here $\Delta_{H 0}$ is dominated by the same sources of uncertainty as the total cross section $\sigma_{\text {total }}$, and hence should be considered $100 \%$ correlated with its uncertainty


Fig. 31: Relative uncertainties for the 0 -jet bin cross section from resummation at NNLL+NNLO for beam thrust $\mathcal{T}_{\mathrm{cm}}$ on the left and $p_{T}^{\text {jet }}$ on the right.
$\Delta_{\text {total }}$. The uncertainty $\Delta_{S B}$ is only present due to the jet-bin cut, and hence gives the $\Delta_{\text {cut }}$ uncertainty that is anti-correlated between neighboring jet bins.

If we simultaneously consider the cross sections $\left\{\sigma_{0}, \sigma_{\geq 1}\right\}$ then the full correlation matrix in method C is

$$
C_{C}=\left(\begin{array}{cc}
\Delta_{S B}^{2} & -\Delta_{S B}^{2}  \tag{98}\\
-\Delta_{S B}^{2} & \Delta_{S B}^{2}
\end{array}\right)+\left(\begin{array}{cc}
\Delta_{H 0}^{2} & \Delta_{H 0} \Delta_{H \geq 1} \\
\Delta_{H 0} \Delta_{H \geq 1} & \Delta_{H \geq 1}^{2}
\end{array}\right),
$$

where $\Delta_{H \geq 1}=\Delta_{\text {total }}-\Delta_{H 0}$ encodes the $100 \%$ correlated component of the uncertainty for the ( $\geq 1$ )jet inclusive cross section. Computing the uncertainty in $\sigma_{\text {total }}$ gives back $\Delta_{\text {total }}$.

Eq. (98) can be compared to $C_{A}$ for method A in Eq. (95), which corresponds to taking $\Delta_{S B} \rightarrow 0$ and obtaining the analog of $\Delta_{H 0}$ by up/down scale variation without resummation ( $\mu_{H}=\mu_{B}=\mu_{S}$ ). It can also be compared to $C_{B}$ for method B in Eq. (97), which corresponds to taking $\Delta_{S B} \rightarrow \Delta_{\geq 1}$ and $\Delta_{H \geq 1} \rightarrow 0$, such that $\Delta_{H 0} \rightarrow \Delta_{\text {total }}$. The numerical dominance of $\Delta_{S B}^{2}$ over $\Delta_{H 0} \Delta_{H \geq 1}$ in the 0 -jet region is another way to justify the preference for using method B when only given a choice between methods A and B. For example, for $p_{T}^{\mathrm{cut}}=30 \mathrm{GeV}$ and $\left|\eta^{\text {jet }}\right| \leq 5.0$ we have $\Delta_{S B}^{2}=0.17$ and $\Delta_{H 0} \Delta_{H \geq 1}=0.02$.

In Fig. 31 we show the uncertainties $\Delta_{S B}$ (light green) and $\Delta_{H 0}$ (medium blue) as a function of the jet-veto variable, as well as the combined uncertainty adding these components in quadrature (dark orange). From the figure we see that the $\Delta_{H 0}$ dominates at large values where the veto is turned off and we approach the total cross section, and that the jet-cut uncertainty $\Delta_{S B}$ dominates for the small cut values that are typical of experimental analyses with Higgs jet bins. The same pattern is observed in the left panel which directly uses the NNLL+NNLO predictions for $\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$, and the right panel which shows the result from reweighting these predictions to $p_{T}^{\mathrm{cut}}$ as explained in Sec .12 .34 below.

### 12.34 Comparison of Uncertainty Methods

In Fig. 32 we compare the uncertainties for the 0 -jet bin cross section from methods A (medium green), B (light green), and C (dark orange). In the upper panels we use $\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$ as the jet-veto variable and full results for the NNLO and NNLL+NNLO cross sections, while in the lower panels we use $p_{T}^{\text {cut }}$ as the jet-veto variable with the full NNLO and the reweighted NNLL+NNLO results (as explained below). The upper panels use a cut on beam thrust, $\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$ while the lower panels use $p_{T}^{\mathrm{cut}}$. The right panels show the same results as those on the left, but are normalized to the highest-order result to better show the relative differences and uncertainties. The uncertainties in methods $\mathrm{A}, \mathrm{B}$, and C are computed from the upper left entry of the matrices $C_{A}, C_{B}$, and $C_{C}$, respectively.


Fig. 32: Comparison of uncertainties for methods A, B, C for the 0 -jet bin cross section for beam thrust $\mathcal{T}_{\text {cm }}$ (top) and $p_{T}^{\text {jet }}$ (bottom). Results are shown at NNLO with uncertainties from methods A and B and for the NNLL+NNLO resummed result using method C (reweighted for $p_{T}^{\mathrm{cut}}$ ). On the right all curves are normalized relative to the NNLL+NNLO central value.

From Fig. 32 we see that in method A (medium green bands) for small values of $p_{T}^{\text {cut }}$ the cancellations that take place in $\sigma_{0}\left(p^{\text {cut }}\right)$ cause the error bands to shrink and eventually almost vanish at $p_{T}^{\text {cut }} \simeq 25 \mathrm{GeV}$, where there is an almost exact cancellation between the two series in Eq. 88). This is avoided by using method B (light green bands). For large values of $p_{T}^{\text {cut }}$ method B reproduces the method A scale variation, since $\sigma_{\geq 1}\left(p^{\text {cut }}\right)$ becomes small. On the other hand, for small values of $p_{T}^{\text {cut }}$ the uncertainties estimated using method B are more realistic, because they explicitly estimate the uncertainties due to the presence of higher order large logarithmic corrections.

The features of this plot are quite generic. In particular, the same pattern of uncertainties is observed for the Tevatron, when using $\mu=m_{H}$ as our central scale (with $\mu=2 m_{H}$ and $\mu=m_{H} / 2$ for the range of scale variation), whether or not we only look at jets at central rapidities, or when considering the exclusive 1 -jet cross section. We also note that using independent variations for $\mu_{f}$ and $\mu_{r}$ does not change this picture, in particular the $\mu_{f}$ variation for fixed $\mu_{r}$ is quite small.

For method C with $\mathcal{T}_{\mathrm{cm}}$ we make use of resummed predictions for $H+0$ jets from gluon fusion at next-to-next-to-leading logarithmic order (NNLL+NNLO) from Ref. [375]. This includes the correct NNLO fixed-order corrections for $\sigma_{0}\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)$ for any cut. The resulting cross section $\sigma_{0}\left(\mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}\right)$ has the jet veto implemented by a cut $\mathcal{T}_{\mathrm{cm}} \leq \mathcal{T}_{\mathrm{cm}}^{\mathrm{cut}}$. This cross section contains a resummation of large logarithms at two orders beyond standard LL parton shower programs. A similar resummation for the case of $p_{T}^{\text {jet }}$ is not available. Instead, we use MC @ NLO and reweight it to the resummed predictions in $\mathcal{T}_{\mathrm{cm}}$, doing so for both the central curve as well as each of the six scale variation curves needed for the uncertainty


Fig. 33: In the left panel we show the same three curves as in the bottom-left panel of Fig. 32, but for the event fraction $f_{0}\left(p_{T}^{\mathrm{cut}}\right)$ treated as a derived quantity from the jet-bin cross sections. In the right panel we contrast the uncertainties obtained using Eqs. (92) and (93) together with method A, with the uncertainty obtained using method B.
determination in method $C{ }^{24}$ We then use the reweighted Monte Carlo sample to obtain cross section predictions for the standard jet veto, $\sigma_{0}\left(p_{T}^{\mathrm{cut}}\right)$. We will refer to this as the reweighted NNLL+NNLO result. Since the Monte Carlo here is only used to provide a transfer matrix between $\mathcal{T}_{\text {cm }}$ and $p_{T}^{\text {jet }}$, and both variables implement a jet veto, one expects that most of the improvements from the higherorder resummation are preserved by the reweighting. However, we caution that this is not equivalent to a complete NNLL+NNLO result for the $p_{T}^{\text {cut }}$ spectrum, since the reweighting may not fully capture effects associated with the choice of jet algorithm and other effects that enter at this order for $p_{T}^{\text {cut }}$. The dependence on the Monte Carlo transfer matrix also introduces an additional uncertainty, which should be studied and is not included in our numerical results. The transfer matrix is obtained at the parton level, without hadronization or underlying event, since we are reweighting a partonic NNLL+NNLO calculation.

From Fig. 32 one observes that the resummation of the large jet-veto logarithms (dark red central curve) lowers the cross section for both $\mathcal{T}_{\mathrm{cm}}^{\text {cut }}$ and $p_{T}^{\text {cut }}$. Comparing to NNLO for cut values $\gtrsim 25 \mathrm{GeV}$ the relative uncertainties in the resummed result of method C (dark orange bands) and the reduction in the resummed central value are similar for both jet-veto variables. Since one expects resummation to decrease the uncertainties, one can also see that the NNLO uncertainties from method B are more consistent with the higher order NNLL+NNLO resummed method C results than those in method A . We observe that the uncertainties in method C are reduced by about a factor of two compared to those in method B. Since the zero-jet bin plays a crucial role in the $H \rightarrow W W$ channel for Higgs searches, and these improvements will also be reflected in uncertainties for the one-jet bin, the improved theoretical precision obtained with method C has the potential to be quite important.

In Fig. 33 we show results for the 0 -jet event fraction $f_{0}$, with $p_{T}^{\text {cut }}$ as the jet-veto variable. In the left panel we compare the uncertainties in $f_{0}\left(p_{T}^{\text {cut }}\right)$ that result from propagating the uncertainties from the jet-bin cross sections obtained from methods A (medium green), B (light green), and C (dark orange). The conclusions are analogous to the corresponding cross-section results in the bottom-left panel of Fig. 32, namely that method B provides a better estimate for the perturbative fixed-order uncertainties than method A, and that the higher-order logarithmic summation present in method C leads to a slightly smaller central value together with the decrease to the uncertainty one expects from incorporating the resummation. In the right panel of Fig. 33 we show the results of the different perturbative schemes for $f_{0}$ defined in Eq. 92) (middle dark green band) and Eq. 93) (lower narrow blue band and upper wide

[^210]|  | method A | method B | method C |
| :---: | :---: | :---: | :---: |
| $\delta \sigma_{0}\left(p_{T}^{\text {cut }}\right)$ | $3 \%$ | $19 \%$ | $9 \%$ |
| $\delta \sigma_{\geq 1}\left(p_{T}^{\text {cut }}\right)$ | $19 \%$ | $19 \%$ | $14 \%$ |
| $\rho\left(\sigma_{\text {total }}, \sigma_{0}\right)$ | 1 | 0.78 | 0.15 |
| $\rho\left(\sigma_{\text {total }}, \sigma_{\geq 1}\right)$ | 1 | 0 | 0.65 |
| $\rho\left(\sigma_{0}, \sigma_{\geq 1}\right)$ | 1 | -0.63 | -0.65 |
| $\delta f_{0}\left(p_{T}^{\text {cut }}\right)$ | $6 \%$ | $13 \%$ | $9 \%$ |
| $\delta f_{\geq 1}\left(p_{T}^{\text {cut }}\right)$ | $10 \%$ | $21 \%$ | $11 \%$ |
| $\rho\left(\sigma_{\text {total }}, f_{0}\right)$ | -1 | 0.43 | -0.38 |
| $\rho\left(\sigma_{\text {total }}, f_{\geq 1}\right)$ | 1 | -0.43 | 0.38 |

Table 9: Example of relative uncertainties $\delta$ and correlations $\rho$ obtained for the LHC at 7 TeV for $p_{T}^{\text {cut }}=$ 30 GeV and $\left|\eta^{\text {jet }}\right| \leq 5.0$.
yellow band) each at NNLO and in each case obtaining the uncertainties using method A (direct scale variation) [376](Sec. 5.3). For comparison, the middle light green band shows the uncertainties obtained from method B. The different method A schemes have a wide spread, which demonstrates the large size of the higher-order perturbative corrections in the total and inclusive 1-jet cross sections. The central values of the alternative methods $A_{2}$ and $A_{3}$ are not covered by the method $A_{1}$ uncertainty band, but all three central curves are covered by the larger uncertainty band from method B (except at small $p_{T}^{\text {cut }}$ where scheme 3 starts to diverge earlier than the other schemes). This can be taken as a confirmation that method A tends to underestimate the perturbative uncertainties in the fixed-order results [376](Sec. 5.3), while method B produces more realistic fixed-order uncertainties.

To appreciate the effects of the different methods on the correlation matrix we consider as an example the results for $p_{T}^{\text {cut }}=30 \mathrm{GeV}$ and $\left|\eta^{\text {jet }}\right| \leq 5.0$. The inclusive cross sections are $\sigma_{\text {total }}=(8.76 \pm$ $0.80) \mathrm{pb}$ at NNLO, and $\sigma_{\geq 1}=(3.31 \pm 0.64) \mathrm{pb}$ at NLO. The relative uncertainties and correlations at these cuts for the three methods are shown in Table 9 . The numbers for the cross sections are also translated into the equivalent results for the event fractions, $f_{0}\left(p_{T}^{\text {cut }}\right)=\sigma_{0}\left(p_{T}^{\text {cut }}\right) / \sigma_{\text {total }}$ and $f \geq 1\left(p_{T}^{\text {cut }}\right)=$ $\sigma_{\geq 1}\left(p_{T}^{\text {cut }}\right) / \sigma_{\text {total }}$. Note that method A should not be used due to the lack of a contribution corresponding to $\Delta_{\text {cut }}$ in this method, and the resulting underestimated $\delta \sigma_{0}$. In methods B and C we see, as expected, that $\sigma_{0}$ and $\sigma_{\geq 1}$ have a substantial anti-correlation due to the jet-bin boundary they share.

### 12.4 Conclusion

To summarize, we have discussed the implications of separating LHC cross sections into jet bins, using Higgs production from gluon fusion as a concrete example. The jet binning induces logarithmic dependences on the jet-bin boundary which is important to properly take into account when making predictions and estimating perturbative uncertainties. When using fixed-order predictions only, the additional logarithms at higher orders in perturbation theory caused by the jet binning can be taken into account in the perturbative uncertainty estimate using method B. By resumming the jet-binning logarithms one can obtain improved predictions with reduced (and more sophisticated) uncertainties using method C.

Here we have focused our discussion on $\sigma_{0}$ and $\sigma_{\geq 1}$ and how to take into account the resulting jet-bin boundary. To further separate $\sigma_{\geq 1}$ into a one-jet bin $\sigma_{1}$ and a $\sigma_{\geq 2}$ one can use method B for this boundary by treating $\Delta_{\geq 2}$ as uncorrelated with the total uncertainty for $\sigma_{\geq 1}$ from either methods B or C. Examples of utilizing method B for this jet bin boundary can be found in Ref. [26]. Once it becomes available one can also use a resummed prediction with uncertainties for this boundary with method C .

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## 13. A NLO BENCHMARK COMPARISON FOR INCLUSIVE JET PRODUCTION AT HADRON COLLIDERS ${ }^{25}$


#### Abstract

We present a benchmark comparison of two next-to-leading order (NLO) calculations for inclusive jet and jet pair production at hadron colliders. A new version of the NLO code EKS is adapted for computation of differential cross sections and compared to an independent calculation based on the FastNLO code. A percent-level agreement between the two codes is observed for specified settings of computations at typical transverse momenta and rapidities of Tevatron and LHC measurements. We identify theoretical prerequisites for achieving such level of agreement and comment on the stability of NLO calculations with respect to the factorization scale choice.


### 13.1 INTRODUCTION

Inclusive jet production at hadron colliders provides an excellent opportunity to test perturbative QCD (PQCD) and look for possible new physics beyond the Standard Model (SM) over a wide range of energy scales. Single inclusive jet production in the Tevatron Run-2 has been recently used to determine the QCD coupling constant [377] and constrain parton distribution functions (PDF) in the proton in global QCD analyses by several groups [255, 378, 262, 311]. Jet production data provide constraints on the gluon PDF at large $x$ values, possibly in a combination with small- $x$ quark PDFs, as discussed in Section 7. Invariant mass distributions of dijets [379], angular distributions [380, 381], and other jet observables at the LHC [382, 293, 292] provide a unprecedented opportunity to extend searches for quark compositeness and new particle resonances toward the highest energies attainable.

In this contribution, we examine agreement between the computer programs that are available for NLO calculations of jet production cross sections. NLO QCD predictions for jet production work remarkably well in a wide kinematical range and across many orders of magnitude of the cross sections. Nonetheless, the latest PDF analysis evaluates many scattering processes up to NNLO in perturbative QCD. Jet production observables are pivotal for constraining the large- $x$ gluon PDF, but remain known to NLO only. We identify and document main factors affecting NLO jet cross sections at a few-percent level of accuracy and compare the numerical results for typical collider kinematics. Differences between the programs used, and choices for the theoretical inputs made, may be responsible for some differences observed between CT10 and other PDFs, as explained below. Such NLO benchmark comparison will be useful for quantifying or reducing the uncertainties on the resulting PDFs and for the future implementation of NNLO and higher-order resummed contributions to the jet cross sections.

From the experimental point of view, jet production has an advantage of very high statistics and a drawback of sizeable systematical errors associated with complexities of jet reconstruction. NLO theoretical uncertainties due to the QCD scale dependence and the fixed-order model for the jet algorithm are comparable to the experimental errors. Control of numerical accuracy involves, in particular, careful tuning of Monte-Carlo integration to handle steeply falling jet cross sections.

An early numerical code (EKS) for the NLO calculation of single-inclusive jet and dijet distributions was developed by S. D. Ellis, Z. Kunszt and D. E. Soper in 1990's [383] based on the subtraction method. Two other widely used numerical programs are NLOJET++ [384, 385] and FastNLO [290, 291].

[^211]The latter provides a fast interface to obtain NLO predictions in kinematical bins of already published experimental jet cross sections by interpolating table files produced by NLOJET++. Besides these fixedorder calculations, POWHEG combines the NLO jet production cross sections with leading-logarithm QCD showering effects [386]. Some phenomenological studies also include partial NNLO contributions to jet cross sections obtained by threshold resummation [387].

The agreement between the above NLO numerical programs is not automatically met, which motivates the present benchmark comparison. The past CTEQ PDF analyses computed NLO jet cross sections using NLO K-factor tables produced by the EKS code, while other PDF analysis groups use FastNLO. Since the CT10 NLO gluon PDF behaves somewhat differently at large $x$ than the gluon PDF from MSTW'08 or other groups [262], one must compare the EKS and FastNLO computations for the same input values to confirm that these programs do not cause the observed disagreement.

Here we show that the results for the Tevatron $(\sqrt{s}=1.96 \mathrm{TeV})$ and LHC $(\sqrt{s}=7 \mathrm{TeV})$ from EKS and FastNLO agree well when the computation parameters are chosen as described in the next section. These settings must be consciously controlled in order to reach acceptable agreement. As a result of this work, the EKS code has been revised to improve its stability and efficiency and to implement output into new differential cross sections [388].

### 13.2 Theoretical setup and inputs

Several theoretical inputs must be matched exactly between the EKS and FastNLO programs in order to reach the level of agreement shown in the figures below.

- Jet algorithm. When calculating the distribution of jet observables, we need to use the same jet algorithms as the ones in the experimental measurements. In this comparison, we utilized the cone-based Midpoint algorithm [389] for the Tevatron observables and cluster-based anti- $k_{T}$ algorithm [341] for the LHC. The only difference between the Midpoint algorithm and modified Snowmass algorithm [389] used in the original EKS program is that the Midpoint algorithm always starts with the middle point between the two partons' directions as a seed for a new protojet, no matter how large their separation is. In the NLO theoretical calculations for single-jet or dijet production that include at most three final-state partons, the cluster-based $k_{T}$ [390], anti- $k_{T}$, and Cambridge-Aachen (CA) [391] algorithms are equivalent.
- The recombination scheme is a procedure for merging two nearby partons into one jet. For example, the energy scheme (4D, based on adding the 4-momentum) or $E_{T}$ scheme (based on adding the scalar $E_{T}$, then averaging over the partons' directions using $E_{T}$ as the weights) can be employed to find the momentum of the merged jet [392]. Our comparison uses the energy scheme for both the Tevatron and LHC measurements, as it is often used by the recent experiments. Different choices of the recombination scheme can cause differences of up to ten percent in the NLO distributions, as will be shown later. Note that, with the energy scheme, the jet could be massive, which means that the jet's pseudorapidity will not be equal to its rapidity.
- The jet trigger imposes acceptance conditions on each jet's $p_{T}$ or rapidity when deciding if this jet's contribution is included into the jet observable. In NLO calculations of single-inclusive jet distributions, the jet trigger conditions have no influence. In dijet production, they may change the cross sections by small amounts by affecting the selection of two leading jets in some cases. In our dijet calculations we choose $p_{T}>40 \mathrm{GeV},|y|<3$ for each jet at the Tevatron and $p_{T}>30 \mathrm{GeV}$, $|y|<3$ at the LHC.
- Renormalization and factorization scales. The scale choice is only related to theory and has no correspondence in experiment. It is conventional to choose the renormalization and factorization scales to be of order of the typical transverse momentum $p_{T}$ of the jet(s): $\mu_{R} \sim \mu_{F} \sim p_{T}$. In contributions with two resolved jets, $p_{T}$ naturally corresponds to the transverse momentum of either of the final-state jets (which are equal by momentum conservation). More ambiguity
is present in contributions with three resolved jets, when $p_{T}$ can correspond to the transverse momentum of either of the jets in each event or to a combination of three transverse momenta. A meaningful comparison must use equivalent definitions of " $j$ et $p_{T}$ " in the renormalization and factorization scales of both NLO calculations.
When FastNLO interpolates tables of NLOJET++ cross sections for single inclusive-jet production, it sets $\mu_{R}$ and $\mu_{F}$ proportional to the $p_{T}$ value at a fixed point in each $p_{T}$ bin of the experimental data. Given the high precision of the latest PDF analyses, the FastNLO scale convention produces a numerically different result than the scale proportional to the $p_{T}$ of the leading jet or the average $p_{T}$ of two leading jets in each event. It depends on the binning of the experimental data and is numerically close to the average $p_{T}$ in each bin for small enough bins.
In the EKS calculations for single-jet production, we set the scale proportional to $p_{T}$ of each individual jet in any $p_{T}$ bin, which means that we repeat the evaluation of the matrix elements with three resolved jets (contributing to three $p_{T}$ bins) by successively setting $\mu_{R, F}$ to be proportional to the $p_{T}$ of each jet in the event. Such matrix elements are thus evaluated three times. This event-level scale setting of EKS turns out to be numerically close to the bin-level scale setting of FastNLO if the bin sizes are small. However, a few-percent differences are still observed at the largest rapidities and $p_{T}$. For dijet production, FastNLO and EKS choose the $\mu_{R}$ and $\mu_{F}$ scales that are proportional to the average $\left|p_{T}\right|=\left(\left|p_{T 1}\right|+\left|p_{T 2}\right|\right) / 2$ of the two leading jets.
- Monte-Carlo integration. Precision calculations for jet production are numerically challenging because of the rapid falloff of the cross sections with the jet's $p_{T}$ and rapidity, and also because of large numerical cancellations occurring between some $2 \rightarrow 2$ and $2 \rightarrow 3$ contributions. Both EKS and NLOJET ++ evaluate differential cross sections by Monte-Carlo integration, which requires to generate of order $10^{9}$ of sample points to achieve percent-level accuracy for the whole kinematical region. The upgraded EKS code performs the Monte-Carlo integration using the VEGAS method from the CUBA2.1 library [393]. The EKS output is produced in the form of two-dimensional cross sections ( $\left.d^{2} \sigma /\left(d p_{T} d y\right), d^{2} \sigma /\left(d M_{j j} d y\right), \ldots\right)$ and stored in finely binned two-dimensional histograms. Such output is "almost fully differential" in the sense that the finely grained histograms can be rebinned into any set of coarse bins of the given experiment at the stage of the user's final analysis. This format is different from the FastNLO format, which provides the cross sections in coarse bins taken from pre-existing experimental publications.
The fine binning in EKS is introduced at the stage of Monte-Carlo integration in order to improve convergence and to better handle the NLO cancellations. The Monte Carlo sampling pattern is tuned automatically to ensure that all fine bins are filled with comparable numbers of sample points, regardless of the momentum and scattering angle values associated with each bin. Then we get uniform relative errors on the cross sections in all bins without consuming too much CPU time, and despite the dramatic variation of cross sections across the bins. Finally, EKS includes a module to allow for flexible choices of scales $\mu_{R}$ and $\mu_{F}$, and another module for calculating differential cross sections of user-provided jet observables.


### 13.3 RESULTS

Figs. 3439 compare our representative numerical results with the ones provided by FastNLO for $p_{T}$ distributions of single jets, invariant mass distributions of dijets, and (in the case of D0 Run-2) angular distributions ( $\chi$ ) of dijets. Kinematical bins of the Tevatron $(\sqrt{s}=1.96 \mathrm{TeV}$ ) [287, 285, 289, 394] and LHC $(\sqrt{s}=7 \mathrm{TeV})$ [293, 292] measurements, and CTEQ6.6 PDFs [256] were used. The cone sizes $R$ of the jets are indicated in the figures.

Left panels in the figures show ratios of EKS to FastNLO cross sections, $\sigma_{\text {EKS }} / \sigma_{\text {FastNLO }}$, at the LO (red points) and $\mathrm{NLO}=\mathrm{LO}+\mathrm{NLO}$ correction (blue points), in kinematical bins provided by the experiments. The horizontal axis indicates the ID of each bin, which are arranged in the order of increasing jet rapidity $y$ and then jet's $p_{T}$ for inclusive jet production, $y$ and then $M_{j j}$ for dijet production, and $M_{j j}$
then $\chi$ for dijet angular dependence. Vertical lines indicate the boundaries of each rapidity interval for single-jet and dijet distributions, and of each dimass interval for the $\chi$ distribution. For example, Fig. 34 shows $\sigma_{\text {EKS }} / \sigma_{\text {FastNLO }}$ in 6 bins of jet rapidity, with bins $1 . . .23$ corresponding to the first rapidity bin ( $|y|<0.4$ ), bins $24 \ldots 45$ corresponding to the second rapidity bin $(0.4<|y|<0.8$ ), and so on.

The left panel includes, from top to bottom, three plots obtained with the renormalization and factorization scales equal to $1 / 2,1$, and 2 times the center scale. We can see a good overall agreement between EKS and FastNLO both at LO and NLO. The only significant discrepancies are found in the highest $p_{T}$ bins for both the Tevatron and LHC single inclusive jet production, which may be due to the difference in the scale choices used in EKS and FastNLO. [These differences reduce when going to NLO]. In the EKS single-jet calculation, we use the actual $p_{T}$ of the partonic jet filled into the bin as the scale input. FastNLO sets the scale according to a fixed $p_{T}$ value in each experimental bin, which tends to be different from the EKS scale in the highest $p_{T}$ bins, which have large widths. The same reason causes a small normalization shift in the other $p_{T}$ bins.

For dijet production, we only observe random fluctuations at highest $M_{j j}$ that are mainly due to numerical integration errors.

In the right panels of Figs. 34 39, we present plots of the NLO K factor from EKS for each distribution, defined as the ratio of the NLO differential cross section to the LO one. The value of the K factor and its stability with respect to the scale choice may provide an indication of the magnitude of yet higher-order corrections.

To minimize the potential effect of higher-order terms, one might opt to choose the renormalization and factorization scales that bring the K factor close to unity in most of the kinematical region. An alternative approach for setting the scale is based on the minimal sensitivity method, which suggests to choose the $\mu_{R}$ and $\mu_{F}$ values (taken to be equal and designated as $\mu$ in the following) at the point where the scale dependence of the NLO cross section is the smallest.

In (di)jet production at central rapidities at the Tevatron, both requirements ( $K \approx 1$ and $d \sigma_{N L O}(\mu) / d \mu \approx 0$ ) could be satisfied by choosing $\mu \approx 0.5 p_{T}$; see, e.g., the appendix in Ref. [395]. For this reason, the scale $p_{T} / 2$ was used in the CT10 study. However, the point of the minimal sensitivity shifts to higher values (close to $p_{T}$ or even higher) at forward rapidities at the Tevatron or at all rapidities at the LHC. For such higher scales, however, it is hard to satisfy the requirement that $K$ remains close to unity at the same time.

This point is illustrated by our plots of the $K$ factors. At the central rapidities and $\mu_{R}=\mu_{F}=$ $0.5 p_{T}$ at the Tevatron (the lowest 3 rapidity bins in Figs. 34.37), $K \approx 1$ and is relatively independent of $p_{T}$, as seen in the top subpanels. However, with this scale choice the K factor deviates significantly from unity and has strong kinematic dependence if the rapidity and $p_{T}$ are large. If one chooses the scale that is equal to $p_{T}$ or even $2 p_{T}$ (the middle and bottom figures), in accord with the minimal sensitivity method for the forward bins, the kinematical dependence of the K factor reduces, but its value increases to 1.3-1.6 in most of the bins.

For CMS kinematics (Figs. 38|39), the $K$ factor has significant kinematical dependence for all central scale choices, however, the choice $\mu_{R}=\mu_{F}=p_{T}$ (the middle subpanels) results in a comparatively flatter $K$ factor that is also closer to unity. We can see that it is hard to find a fixed scale (or a scale of the type $p_{T} \times($ a function of $y)$ [383]) that would simultaneously reduce the magnitude of the NLO correction and stabilize its scale dependence and kinematical dependence. The scale $0.5 p_{T}$ may be slightly more optimal at the Tevatron, and the scale $p_{T}$ may be slightly better at the LHC. In the absence of a clearly superior scale choice, it may be necessary to vary the scale of jet cross sections in the global fit in order to estimate its effect on the PDF errors.

In Figs. 40 and 41, we plot the ratios of the NLO distributions calculated using different recombination schemes, where $\sigma_{4 D}$ is obtained with the energy scheme, and $\sigma_{E_{T}}$ is with the $E_{T}$ scheme. For single inclusive jet production at both the Tevatron and LHC, $\sigma_{E_{T}}$ is larger then $\sigma_{4 D}$. An opposite trend
is observed in dijet production. Differences of the predictions based on the two schemes are larger with the Midpoint algorithm (used at the Tevatron) than with the anti- $k_{T}$ algorithm (used at the LHC). In an NLO calculation, the Midpoint algorithm allows a larger maximal angular separation $(2 R)$ between the two partons forming a jet, compared to the anti- $k_{T}$ algorithm that only allows the angular separation up to $R$. This produces the shown kinematical differences between the two schemes.

## CONCLUSIONS

Jet production plays an important role at hadron colliders and is a main background process in the bulk of new physics searches. A benchmark comparison of NLO QCD predictions for jet production from different numerical codes can be useful for both the ongoing phenomenological studies and upcoming higher-order calculations. In this work we modify the original EKS program and compare the singlejet and dijet cross sections that it produces with the ones from the FastNLO program. We find a good agreement between two programs, apart from differences of up to $5-10 \%$ occuring at the highest jet $p_{T}$ 's and rapidities. We document the exact combination of theoretical settings in EKS that are needed to reproduce the FastNLO results. Based on the EKS calculation, we attempted to identify the choice of the renormalization and factorization scales that could simultaneously reduce the magnitude of NLO $K$ factors and/or scale dependence of the NLO cross section. Since we could not easily find such a scale combination, we propose to vary the factorization and renormalization scales in future (N)NLO PDF fits to better estimate theoretical uncertainties in the resulting PDFs. There is a plan to publish the updated EKS program in the near future [388].

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Fig. 34: Comparison of $p_{T}$ distributions for single inclusive jet production from EKS and FastNLO for D0 Tevatron Run II measurement.[287]


Fig. 35: Comparison of $p_{T}$ distributions for single inclusive jet production from EKS and FastNLO for CDF Tevatron Run II measurement. [285]


Fig. 36: Comparison of invariant mass distributions for dijet production from EKS and FastNLO for D0 Tevatron Run II measurement.[289]


Fig. 37: Comparison of angular $(\chi)$ distributions for dijet production from EKS and FastNLO for D0 Tevatron Run II measurement.[394]


Fig. 38: Comparison of $p_{T}$ distributions for single inclusive jet production from EKS and FastNLO for CMS LHC ( 7 TeV ) measurement. [292]


Fig. 39: Comparison of invariant mass distributions for dijet production from EKS and FastNLO for CMS LHC ( 7 TeV ) measurement. [293]


Fig. 40: Comparison of $p_{T}$ distributions for single inclusive jet production using different recombination schemes.


Fig. 41: Comparison of invariant mass distributions for the dijet production using different recombination schemes.

## 14. PHENOMENOLOGICAL STUDIES WITH AMC@ NLO ${ }^{26}$


#### Abstract

We present four phenomenological studies of hadron collider processes performed within the aMC @ NLO framework


### 14.1 Introduction

aMC@NLO (http://amcatnlo.cern.ch) is a fully automated approach to complete event generation and subsequent parton shower at the NLO accuracy in QCD, which allows accurate and flexible simulations for both signals and backgrounds at hadron colliders. All calculational aspects in aMC @ NLO are automated. One-loop contributions are evaluated with MadLoop [8, 396], that uses the OPP integrand reduction method [121] as implemented in CutTools [135]. The other matrix-element contributions to the cross sections, their phase-space subtractions according to the FKS formalism [397], their combinations with the one-loop results, and their integration are performed by MadFKS [398] ${ }^{27}$. The matching of the NLO results with HERWIG [399] or PYTHIA [400] parton showers is performed with the MC@NLO method [401], and it is also completely automatic. Finally, aMC @ NLO can compute scale and PDF uncertainties at no extra CPU-time cost with the help of the process-independent reweighting technique described in [402].

For all technical details we refer to the original publications. We report here on the physics results obtained with aMC @ NLO for observables of interest at hadron colliders [15, 403, 402, 404]. We stress that they are simulated at the hadron level, namely including parton shower and hadronization effects. In Sects. 14.2, 14.3, and 14.4 we present results for the production of $t t H, V b b$, and four-lepton final states at the LHC, respectively. Section 14.5 reports on a study of the $W j j$ process at Tevatron. Finally, in sect. 14.6 we draw our conclusions. The list of the processes considered here should convince the reader that one can perform realistic analyses of experimental data, for signals and backgrounds, entirely within the aMC@NLO framework.

### 14.2 The $t t H$ process at the LHC

The production process of a $H$ boson in association with a top pair [15] is a classic mechanism for Higgs production at the LHC [24, 405], where the large $t t H$ Yukawa coupling and the presence of top quarks can be exploited to extract the signal from its QCD multi-jet background. As an example of the use of aMC @ NLO for this process we present, in Fig. 42, the Higgs transverse momentum distribution and the transverse momentum of the $t t H$ or $t t A$ system at the $\sqrt{s}=7 \mathrm{TeV}$ LHC for a Standard Model (scalar) Higgs with $M_{H}=120 \mathrm{GeV}$ and for a pseudoscalar one with $M_{A}=120 / 40 \mathrm{GeV}$. The total NLO cross sections in the three cases are $\sigma_{\mathrm{NLO}}\left(M_{H}=120\right)=103.4 \mathrm{fb}, \sigma_{\mathrm{NLO}}\left(M_{A}=120\right)=31.9 \mathrm{fb}$, and $\sigma_{\mathrm{NLO}}\left(M_{A}=40\right)=77.3 \mathrm{fb}$, respectively. At moderate values of the Higgs transverse momentum, the scalar and pseudoscalar cases are clearly distinguishable, while at larger values the three distributions tend to coincide. Parton shower effects give in general small corrections with respect to the a pure NLO calculation, except for variables involving all produced particles, such as the transverse momentum of the $t t H$ or $t t A$ system shown in the right panel of Fig. 42.

### 14.3 The $V b b$ process at the LHC

With $V b b$ we understand $\ell \nu b b$ and $\ell^{+} \ell^{-} b b$ final states [403], which are the main backgrounds to searches for SM Higgs production in association with vector bosons $(W H / Z H)$, with the subsequent Higgs decay into a $b b$ pair. The aMC @ NLO framework allows a realistic study including

- NLO corrections;

[^212]

Fig. 42: Higgs transverse momentum distributions (left) and transverse momentum of the $t t H$ or $t t A$ system (right) in $t t H / t t A$ events at the LHC ( $\sqrt{s}=7 \mathrm{TeV}$ ), with aMC @ NLO in the three cases: Scalar (blue) and pseudoscalar (magenta) Higgs with $m_{H / A}=120 \mathrm{GeV}$ and pseudoscalar (green) with $m_{A}=$ 40 GeV . In the lower panels of the left part, the ratios of aMC @ NLO over LO (dashed), NLO (solid), and aMC@LO (crosses) are shown. Solid histograms in the right panel are relevant to aMC@NLO, dashed ones to a pure NLO calculation.

- bottom quark mass effects;
- spin-correlation and off-shell effects;
- showering and hadronization.

As an example we show, in Fig. 43, the invariant mass of the pair of the two leading b-jets, compared with the signal distributions for a standard Higgs with $m_{H}=120 \mathrm{GeV}$. Fig. 43 is interesting because both signal and background are studied at the NLO accuracy. It should be noted that, since completely hadronized events are simulated, sophisticated studies of the jet sub-structure are possible within the aMC@NLO framework, as presented in Fig. 44 , where the fractions of events containing zero $b$-jets, exactly one $b$-jet, and exactly two $b$-jets are plotted. The $b$-jet fractions are fairly similar for $W b b$ and $Z b b$ production, and the effects of the NLO corrections are consistent with the fully-inclusive $K$ factors. On the other hand, the $b b$-jet contribution to the $b$-jet rate is seen to be more than three times larger for $\ell^{ \pm} \nu b b$ than for $\ell^{+} \ell^{-} b b$ final states. This fact is related to the different mechanisms for the production of a $b b$ pair in the two processes. At variance with the case of $\ell^{ \pm} \nu b b$ production, in a $\ell^{+} \ell^{-} b b$ final state the two $b$ 's may come from the separate branchings of two initial-state gluons, and thus the probability of them ending in the same jet is much smaller than in the case of a $g \rightarrow b b$ final-state branching, which gives the only possible contribution to a $\ell^{ \pm} \nu b b$ final state.

### 14.4 Four-lepton production at the LHC

Vector boson pair production is interesting in at least two respects. Firstly, it is an irreducible background to Higgs signals, in particular through the $W^{+} W$ and $Z Z$ channels which are relevant to searches for a standard model Higgs of mass larger than about 140 GeV . Secondly, di-boson cross sections are quite sensitive to violations of the gauge structure of the Standard Model, and hence are good probes of scenarios where new physics is heavy and not directly accessible at the LHC, yet the couplings in the vector boson sector are affected. We consider here the neutral process [402]

$$
p p \rightarrow\left(Z / \gamma^{*}\right)\left(Z / \gamma^{*}\right) \rightarrow \ell^{+} \ell^{-} \ell^{(\prime)+} \ell^{(\prime)-},
$$



Fig. 43: Invariant mass of the pair of the two leading $b$-jets. $W H(\rightarrow \ell \nu b b), Z H\left(\rightarrow \ell^{+} \ell^{-} b b\right), \ell \nu b b$, and $\ell^{+} \ell^{-} b b$ results are shown, with the former two rescaled by a factor of ten.

| Process | Cross section (fb) |  |  |
| :---: | :---: | :---: | :---: |
|  | $q \bar{q} / q g$ channels |  |  |
|  | $\mathcal{O}\left(\alpha_{s}^{0}\right)$ | $\mathcal{O}\left(\alpha_{s}^{0}\right)+\mathcal{O}\left(\alpha_{s}\right)$ | $g g$ channel |
| $p p \rightarrow e^{+} e^{-} \mu^{+} \mu^{-}$ | 9.19 | $12.90_{-0.23(1.8 \%)-0.22(1.7 \%)}^{+0.27(2.1 \%)+0.26(2.0 \%)}$ | $0.566_{-0.118(20.8 \%)-0.014(2.5 \%)}^{+0.162(28.5 \%)+0.012(2.1 \%)}$ |
| $p p \rightarrow e^{+} e^{-} e^{+} e^{-}$ | 4.58 | $6.43_{-0.13(2.0 \%)-0.10(1.6 \%)}^{+0.13(2.1 \%)+0.1(1.7)}$ |  |

Table 10: Total cross sections for $e^{+} e^{-} \mu^{+} \mu^{-}$and $e^{+} e^{-} e^{+} e^{-}$production at the $\mathrm{LHC}(\sqrt{S}=7 \mathrm{TeV})$ within the cuts $M\left(\ell^{ \pm} \ell^{(1) \mp}\right) \geq 30 \mathrm{GeV}$. The first and second errors affecting the results are the scale and PDF uncertainties (also given as fractions of the central values).
which, although smaller than the $W^{+} W^{-}$channel, may provide a cleaner signal due to the possibility of fully reconstructing the decay products of the two vector bosons. aMC @ NLO predictions for the cross sections are given in Tab. 10, which also includes aMC @ NLO estimates for scale and PDF uncertainties. The four-lepton invariant mass and the transverse momentum distribution are presented in Fig. 45, where comparisons between the results obtained with aMC @ NLO matched to HERWIG and to PYTHIA are also given. We stress that these results include the contributions due to $g g$-initiated processes, which have also been computed automatically. These are formally of NNLO, but may play a non-negligible phenomenological role owing to their parton-luminosity dominance at a large-energy collider such as the LHC.

### 14.5 Wjj at Tevatron

In [406] CDF reported an excess of events in two-jet production in association with a $W$ boson, in the form of a broad peak centered at $M_{j j}=144 \mathrm{GeV}$ in the dijet invariant mass ${ }^{28}$. Motivated by this fact, we present in Fig. 46]the aMC @ NLO prediction [404] for the dijet invariant mass in $W j j$ events, using the same cuts as CDF and D0 in the signal region, also comparing with a pure NLO computation and with the Alpgen [408] findings (one-, two-, and three-parton multiplicities have been consistently matched to

[^213]

Fig. 44: Fractions of events (in percent) that contain: zero $b$-jets, exactly one $b$-jet, and exactly two $b$-jets. The rightmost bin displays the fraction of $b$-jets which are $b b$-jets. The two insets show the ratio of the aMC @ NLO results over the corresponding NLO (solid), aMC @ LO (dashed), and LO (symbols) ones, separately for $W b b$ (upper inset) and $Z b b$ (lower inset) production.
obtain the latter). Perturbative, parton-level results agree well with those obtained after shower, and PDF and scale uncertainties (also reported in Fig. 46) are well under control. In summary, we do not observe any significant effects in the shape of distributions due to NLO corrections, which therefore cannot be responsible for the excess of events observed by the CDF collaboration.

### 14.6 Conclusions

The results we have presented in this contribution are based on the strategic assumption that, for the word automation to have its proper meaning, the only operation required from a user is that of typing-in the process to be computed, and other analysis-related information (such as final-state cuts). In particular, the codes that achieve the automation may only differentiate between processes depending on their general characteristics, but must never work on a case-by-case basis. The aMC@NLO framework is based on such an assumption, providing a very powerful tool to compare, at the NLO accuracy including showering and hadronization, theory and experiment in high energy collisions. As an example of the flexibility of aMC@NLO we have presented results for the processes $p p \rightarrow t t H, p p \rightarrow V b b, p p \rightarrow$ $\ell^{+} \ell^{-} \ell^{(1)+} \ell^{(1)-}$ at the LHC, and a study of $p \bar{p} \rightarrow W j j$ at Tevatron.

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## 15. PROBING CORRECTIONS TO DIJET PRODUCTION AT THE LHC ${ }^{29}$

## Abstract

We compare and discuss a few kinematic distributions for dijet production at the LHC, computed with a fixed next-to-leading order code, with the

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Fig. 45: Four-lepton invariant mass and the transverse momentum distributions for aMC@NLO $+g g$ HERWIG (solid black) and PYTHIA (dashed blue) results. The rescaled $g g$ contributions with HERWIG (open black boxes) and PYTHIA (open blue circles) are shown separately. Middle insets: scale (dashed red) and PDF (solid black) fractional uncertainties. Lower insets: aMC@NLO/(aMC@NLO+gg) with HERWIG (solid black) and PYTHIA (dashed blue).

POWHEG BOX and with HEJ. Previous experimental studies have dealt with kinematic distributions where the predictions of the three approaches were very similar. In this proceeding, we investigate kinematic distributions where the resummed effects in POWHEG and HEJ are clearly shown and enhanced with respect to the fixed NLO result, since different QCD-radiation regimes are probed.

### 15.1 Introduction

Dijet production is one of the cornerstone processes at the LHC. The cross section for jet production is very large, making it an important testing ground for our understanding of QCD at high-energy scales. In addition, jet production is an important background for many searches for new physics. It is therefore essential to probe and test our theoretical predictions. Dijet-production studies can bring insights in jet production in association with other particles too: for example, Higgs boson production plus two jets in gluon fusion, a key process for assessing the CP properties of the Higgs boson, can benefit from these studies.

There have been a number of very interesting experimental studies in dijet production by both the ATLAS [410, 411, 294] and CMS [412, 413, 414, 415] Collaborations. It is already clear that higher order QCD contributions beyond a fixed order, low multiplicity calculation can be important because the large available phase space for jet emission at the LHC compensates for the suppression of extra powers of the strong coupling constant.

In this contribution, we compare two theoretical approaches to dijet production that include higher order effects: POWHEG [416, 417, 386, 13] and HEJ [418, 419, 64]. The POWHEG method successfully merges a fixed next-to-leading order (NLO) calculation with a parton shower program, that resums leading logarithmic contributions from collinear emissions. In this study, the POWHEG results obtained with the POWHEG BOX [13] are interfaced with the transverse-momentum-ordered shower


Fig. 46: Invariant mass of the pair of the two hardest jets, with CDF/D0 cuts of [406] (left) and of [409] (right).
provided by PYTHIA 6.4.21 [400]. In contrast, the starting point for HEJ is an all-order approximation to the hard scattering matrix element in the regime of wide-angle QCD emissions. HEJ is accurate at leading logarithmic precision in the invariant mass of any two jets. This is then supplemented with the missing contributions (through a merging and reweighting-procedure) necessary to also ensure tree-level accuracy for final states with up to four jets. The tree-level matrix elements are taken from Standalone Madgraph [163].

The POWHEG and HEJ approaches are clearly very different in their description of QCD radiation. Nevertheless, for several kinematic distributions (see for example ref. [410]) the predictions from POWHEG and HEJ are very similar. In this study, we investigate various observables which can expose the differences in the two approaches and we compare them with the fixed NLO results.

### 15.2 A comparison between NLO, POWHEG and HEJ in dijet production

In order to avoid biasing our event sample, we impose a minimal set of cuts, avoiding symmetric cuts on the jet transverse momenta that would give an unphysical cross section at fixed NLO level [420, 421], due to the presence of unresummed logarithms. Neither the POWHEG or HEJ descriptions suffer from this instability. However, in order to have a sensible fixed NLO cross section to compare with, we impose asymmetric cuts

$$
\begin{equation*}
p_{\mathrm{T}}^{j}>35 \mathrm{GeV}, \quad p_{\mathrm{T}}^{j_{1}}>45 \mathrm{GeV}, \quad\left|y_{j}\right|<4.7, \tag{99}
\end{equation*}
$$

i.e. all jets are required to have a minimum transverse momentum of 35 GeV , and the hardest-jet transverse momentum, $p_{\mathrm{T}}^{j_{1}}$, is required to be greater than 45 GeV . In order to comply with the experimental acceptance, all jets are further required to have an absolute rapidity $\left|y_{j}\right|$ less than 4.7. Jets are defined according to the anti-kt jet algorithm, with radius $R=0.5$. Only events with at least two jets fulfilling Eq. (99) are kept.

In the following, we compare the fixed NLO cross section with the POWHEG first emission results, with the POWHEG results showered by PYTHIA and with the HEJ predictions. The renormalization and factorization scales have been chosen equal to the transverse momentum of the hardest jet in each event, for the HEJ predictions. For the NLO computation (and for computing the POWHEG $\bar{B}$ function), scales are set to the transverse momentum of the so called underlying Born configuration. Scale-uncertainty bands obtained by varying these scales by a factor of two in each direction are shown for the NLO and HEJ results. The scales entering in the evaluation of parton distribution functions and


Fig. 47: The average number of jets as a function of $\Delta y_{\mathrm{fb}}$ (left plot) and of $H_{\mathrm{T}}$ (right plot), as predicted by a fixed NLO calculation, by POWHEG first emission, by POWHEG+PYTHIA and by HEJ. The dotted red lines around the HEJ prediction and the green ones around the NLO result are obtained by varying the renormalization and factorization scales by a factor of two around their central value.
of the strong coupling in the POWHEG Sudakov form factor are instead evaluated with a scale equal to the transverse momentum of the POWHEG hardest emission [417, 386].

In Fig. 47 we plot the average number of jets as a function of the rapidity difference between the most forward and most backward of the jets fulfilling Eq. (99), $\Delta y_{f b}$, on the left-hand side, and as a function of $H_{\mathrm{T}}=\sum_{j} p_{\mathrm{T}}^{j}$ on the right-hand side. The wide-angle resummation implemented in HEJ produces more hard jets than POWHEG and the fixed NLO calculation, as the rapidity separation between the most forward and the most backward jet in the event increases. Both the NLO and the firstemission POWHEG results have at most 3 jets, so that the average number of jets cannot exceed 3 , and give similar results. Additional jets are instead produced by the PYTHIA shower, so that the average number of jets is increased by roughly $20 \%$ with respect to the NLO one, for $\Delta y_{\mathrm{fb}} \approx 7$. For the same separation in rapidity, the HEJ prediction is $45 \%$ larger than the NLO result, with a chance to distinguish among the three approaches.

The dependence of the average number of jets from $H_{\mathrm{T}}$ (right plot) displays a different behaviour: here the showered events have on average more jets than HEJ and the NLO results, as the sum of the transverse momentum of all the final-state jets increases. It is interesting here to comment on the NLO result obtained with the factorization and renormalization scales set to $p_{\mathrm{T}}^{\mathrm{UB}} / 2$, i.e. half of the transverse momentum of the underlying Born configuration. In fact, from the plot, an unphysical behaviour of this quantity emerges: the average number of jets is greater than 3 above $H_{\mathrm{T}} \approx 270 \mathrm{GeV}$. This is due to the fact that the high $H_{\mathrm{T}}$ region is populated mostly by events with 3 jets, two of which have approximately the same high transverse momentum, and the third one is softer with respect to the other two (the cuts in Eq. (99) are always in place). In this configuration, the exclusive two-jet cross section becomes negative, due to incomplete cancellation of the virtual (negative) contribution, now enhanced by a higher value of the strong coupling constant, evaluated at a lower renormalization scale. A more detailed discussion can be found in ref. [422].

As a last example of a kinematic distribution that displays different behaviour if evaluated at NLO or using POWHEG or HEJ, we plot in Fig. 48 the average value of $\cos \left(\pi-\phi_{\mathrm{fb}}\right)$, where $\phi_{\mathrm{fb}}$ is the azimuthal angle between the most forward and backward jets, as a function of their rapidity separation $\Delta y_{\mathrm{fb}}$. For dijet events at tree-level, $\phi_{\mathrm{fb}}=\pi$ since the two jets must be back-to-back, and the average value of the cosine is 1 . Deviation from 1 then indicates the presence of additional emissions, so that


Fig. 48: The average value of $\cos \left(\pi-\phi_{\mathrm{fb}}\right)$ as a function of $\Delta y_{\mathrm{fb}}$, where $\phi_{\mathrm{fb}}$ is the azimuthal angle separation between the most forward and most backward jet. The dotted red and green lines are obtained by varying the renormalization and factorization scales by a factor of 2 in both directions.
this kinematic distribution carries information on the decorrelation between the two jets. This quantity is more inclusive than the average number of jets as it is sensitive also to emissions below the jet $p_{\mathrm{T}}$ cut. The higher radiation activity in POWHEG+PYTHIA and in HEJ, with respect to the fixed NLO and the POWHEG first-emission results, is clearly visible in the figure: the stronger jet activity produced by HEJ at higher rapidity separation (see the left plot of Fig. 47) lowers the average value of the cosine below the POWHEG+PYTHIA result. As expected, the average value predicted by the POWHEG first-emission and the NLO calculation is closer to 1 , since they contain at most one radiated parton.

## Conclusions

In this proceeding, we have discussed the results obtained using a fixed NLO calculation, HEJ and POWHEG+PYTHIA, in the description of three kinematic distributions, selected in order to display more clearly the differences among the three approaches: the average number of jets and azimuthal decorrelation between the most forward and the most backward jet, plotted as a function of the rapidity separation of the most forward and the most backward jet, and the average number of jets plotted as a function of the sum of the transverse momenta of all the jets in the event.

While the limitations of the NLO calculation are clearly visible when we probe regions of the phase space where multi-jet emissions becomes important, the predictions of POWHEG+PYTHIA and HEJ are distinguishable when dealing with the average number of jets as a function rapidity span. Less marked differences are found as a function of Ht , and in the study of the azimuthal decorrelation of the most forward and backward jet.

An experimental analysis of the dijet data, collected at the LHC, should then follow to investigate to which extent our theoretical knowledge for these kinematic distributions is under control.

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## 16. W+JETS PRODUCTION AT THE LHC: A COMPARISON OF PERTURBATIVE TOOLS 30


#### Abstract

In this contribution, we discuss several theoretical predictions for $W$ plus jets production at the LHC, compare the predictions to recent data from the ATLAS collaboration, and examine possible improvements to the theoretical framework.


### 16.1 Motivation

Experimentalists are reliant on a number of tools, at LO and NLO, at parton level and at hadron level, in order to understand both simple and complex final states at the LHC. One of the benchmark processes, for both signals to new physics and for their backgrounds, is the production of $W$ plus jets. In this contribution, we discuss several different predictions for the $W$ plus jets final state, concentrating on the $H_{T}$ distribution. We examine where the predictions agree, and where they disagree and compare the predictions to LHC data. We introduce the idea of NLO 'Exclusive Sums', and discuss the performance of this technique and consider also how LoopSim may be able to improve the predictions. We document the use of ROOT ntuples for $W$ plus jets predictions produced by the BlackHat+Sherpa collaboration, indicating how they can be used to examine the variation of the cross sections with jet size/algorithm, PDFs, and scale choices. We also study the possibility of using the LoopSim method together with BlackHat+Sherpa type ntuples, since this may offer the opportunity to improve on the results from NLO Exclusive Sums.

### 16.2 Theory tools: strengths and weaknesses

NLO is the first order at which the normalization (and sometimes the shape) of LHC cross sections can be realistically calculated. The state of the art is in parton-level programs such as BlackHat+Sherpa, where $W+n$-jet cross sections are available, with $n$ up to 4 at NLO [70, 51, 22] (and soon up to 5 [423]). Of course, such parton-level final states do not allow for the full comparisons to the data allowed by the full parton shower Monte Carlo programs such as Sherpa. NLO matrix elements have been included into parton shower Monte Carlos, but only for relatively simple final states (although we note that the NLO matrix elements for $W+2$ jets [404] and $W+3$ jets [424] have recently been implemented in parton shower Monte Carlo programs).

The Sherpa Monte Carlo program [146, 425] includes the exact LO $W+n$-parton ( $W+n$ jet) matrix elements, with $n$ up to 4 (in this study), using the newer ME\&TS scheme as introduced in Refs. [426, 427, 428] for the addition of states with different jet multiplicities with the correct normalizations. The newer matrix-element plus parton-shower merging scheme improves over the CKKW [429, 430] formalism by allowing for a better interplay between the matrix-element and partonshower descriptions. This in particular required the implementation of truncated showers ('TS'). As before, additional jets are, of course, then produced by the parton shower. Both BlackHat+Sherpa and Sherpa rely on DGLAP-based evolution of gluon emission, on the assumption that the gluon emissions are strongly ordered in transverse momentum. For an alternative prediction, we use the program HEJ [418, 419, 431]. The High Energy Jets (HEJ) framework provides a leading-log resummation of the dominant terms in the limit of large invariant mass between jets. In addition, HEJ contains a merging procedure to ensure tree-level accuracy for final states with two, three or four jets.

[^215]A NLO $n$-jet prediction produces events with with either $n$ or $n+1$ partons. For observables for which higher multiplicities have a significant impact, this limitation can be detrimental. If one has predictions for different multiplicities, one can try to combine them by avoiding double counting by requiring that the $n$-jet prediction is used only to describe $n$-jet events (except for the highest multiplicity where ( $n+1$ )-jets configurations are allowed). This procedure is crude and does not increase the formal accuracy of the prediction which is that of NLO of the smallest multiplicity. The idea is that, in observables where higher multiplicities events dominate, a better prediction might be obtained. This has been denoted as the 'Exclusive Sums' technique. The impact of the Exclusive Sums approach depends on the kinematic variable under consideration. For this contribution, we consider only the $H_{T}$ variable, defined as the sum of the transverse momenta of all of the leptons (including neutrinos) and jets in the event. The impact of the approach is expected to depend on the observable under consideration and it may be more beneficial for variables sensitive to multi-jet radiation, such as $H_{T}$, than for more inclusive variables such as $p_{t, W}$. Comparisons for the latter are left to a study now in progress.

### 16.3 Use of BlackHat+Sherpa ntuples

As has been partially detailed in these proceedings, there have been many advances in the computation of the NLO corrections for multi-parton final states. Often such calculations do not exist in a compact user-friendly form, and other means must be taken to allow experimentalists to have access to the results. The BlackHat+Sherpa collaboration has chosen to make available ROOT tuples that contain all of the parton-level information needed to form flexible predictions. The ROOT ntuple framework is a very efficient way to store such information and the use of ROOT tuples is very familiar to experimentalists.

The ROOT ntuples store the four-vectors for the final state partons, as well as their flavor information. The calculation is originally performed using a specific choice of PDF, $\alpha_{s}\left(m_{Z}\right)$, renormalization scale $\mu_{R}$ and factorization scale $\mu_{F}$, but weight information is also stored in the ntuples that allows each event to be easily re-weighted to any other (reasonable) values for the above parameters. (PDFs are varied through calls to LHAPDF [432].) No jet clustering has been performed on the final state partons; jet reconstruction is left to the user, for any jet algorithm/size for which the correct counter-events are present in the ntuple. For the results presented here, the SISCone [433], $k_{T}$ [361] and anti- $k_{T}$ [341] algorithms, with jet radii $R$ of $0.4,0.5,0.6$ and 0.7 can be used. Each of the above jet algorithms were run and the results stored in SpartyJet ntuples ${ }^{31}$ The SpartyJet tuples were 'friended' with the BlackHat+Sherpa ntuples, allowing the analysis script access to all jet information. Such a flexibility allows for an investigation of the dependence of the physics on the details of the manner in which the partons are combined into jets, in a manner difficult to achieve prior to this.

The four-vector information stored in the BlackHat+Sherpa ntuples is shown in Table 11. Note the variety of entries needed for the re-weighting of the cross section results, especially for the case of the variation of the two scales $\mu_{R}$ and $\mu_{F}$. Information is stored in separate ntuples for the different categories of events, which are typically Born, loop (leading color and sub-leading color), real and subtraction terms. For large $n$, in $W+n$-parton final states, there are many divergences present when two partons become collinear or one parton becomes soft. These divergences are controlled using the traditional Catani-Seymour approach [236], which involves the generation of many counter-events. Many of the events have negative weights; only the sum is guaranteed to be positive-definite. Predictions with reasonable statistical precision may require the sum of billions of events. The resultant tuples may amount to several Terabytes. However, the output can be subdivided into ROOT files of order 5-10 GB, allowing for simultaneous parallel processing of the events over multiple nodes, such as in the Tier3 facility at Michigan State University used for these comparisons.

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### 16.4 BlackHat+Sherpa predictions

We have generated NLO predictions with the BlackHat+Sherpa predictions implementing the cuts used in the 2010 ATLAS $W$ plus jets paper [436]. For completeness, the cuts are reproduced below:

- $p_{T}^{\text {lepton }}>20 \mathrm{GeV}$,
- $\left|\eta^{\text {lepton }}\right|<2.4$,
- $E_{T}^{\text {miss }}>25 \mathrm{GeV}$,
- $m_{T, W}>40 \mathrm{GeV}$,
- $p_{T}^{\text {jet }}>30 \mathrm{GeV}$,
- $\left|y^{\text {jet }}\right|<4.4$,
- $\Delta R^{\text {lepton-jet }}>0.5$.

In Figure 49, we show the NLO BlackHat+Sherpa prediction for the $H_{T}$ distribution for $W+\geq 1$ jets (left) using the anti- $k_{T}$ jet algorithm with $R=0.4$. As the prediction is an inclusive NLO calculation for $W+\geq 1$ jets, there are contributions from both the one-jet and the two-jet final states. Note that as $H_{T}$ increases, the contributions from the $W+2$-jet subprocess also increases. On the right, we again show the $H_{T}$ distribution, but now compute the prediction using the 'Exclusive Sums' technique, adding in the NLO $W+2$-jet information. Now there is a significant contribution at high $H_{T}$ from the $W+3$ -

| branch name | type | notes |
| :---: | :---: | :---: |
| id | I | id of the event. Real events and their associated counter-terms share |
| nparticle | I | number of particles in the final state |
| px | F[nparticle] | array of the x components of the final state particles |
| py | F[nparticle] | array of the $y$ components of the final state particles |
| pz | F[nparticle] | array of the z components of the final state particles |
| E | F[nparticle] | array of the energy components of the final state particles |
| alphas | D | $\alpha_{s}$ value used for this event |
| kf | I | PDG codes of the final state particles |
| weight | D | weight of the event |
| weight2 | D | weight of the event to be used to treat the statistical errors correctly in the real part |
| me_wgt | D | matrix element weight, the same as weight but without pdf factors |
| me_wgt2 | D | matrix element weight, the same as weight2 but without pdf factors |
| x 1 | D | fraction of the hadron momentum carried by the first incoming parton |
| x 2 | D | fraction of the hadron momentum carried by the second incoming parton |
| x1p | D | second momentum fraction used in the integrated real part |
| x2p | D | second momentum fraction used in the integrated real part |
| id1 | I | PDG code of the first incoming parton |
| id2 | I | PDG code of the second incoming parton |
| fac_scale | D | factorization scale used |
| ren_scale | D | renormalization scale used |
| nuwgt | I | number of additional weights |
| usr_wgts | D[nuwgt] | additional weights needed to change the scale |

Table 11: Branches in a BlackHat+Sherpa ROOT file.


Fig. 49: The $W$ plus jets cross section, as a function of $H_{T}$, for the NLO inclusive $W+\geq 1$-jet prediction (left) and for the Exclusive Sums approach, adding in $W+2$-jet production at NLO (right). The cross sections have been evaluated at a central scale of $H_{T} / 2$ and the uncertainty is given by varying the renormalization and factorization scales independently up and down by a factor of 2 , while ensuring that the ratio of the two scales is never larger than a factor of 2 .
jet final state as well. In Figure 50, the $H_{T}$ prediction is shown using the Exclusive Sums approach, adding $1+2+3$ jets at NLO (left) and $1+2+3+4$ jets at NLO (right). It is evident that as $H_{T}$ increases, contributions from higher jet multiplicities that are only present implicitly in a traditional inclusive NLO $W+\geq 1$-jet calculation, become important. The Exclusive Sums $H_{T}$ predictions agree with that for the inclusive NLO $W+\geq 1$-jet calculation at low $H_{T}$, but are larger at higher $H_{T}$, and in better agreement with the ATLAS data (as discussed below).

However, it can also be noticed that the scale dependences for the Exclusive Sums predictions apparently get better when the 2 -jet NLO information is added, but significantly worse when the 3 -jet and 4 -jet information is added. As discussed in the Appendix, the reduction in scale dependence with the addition of the 2-jet NLO terms may be due to the stabilization of the predictions for the $q q \rightarrow W q^{\prime} q$ topologies. Adding the 3 -jet and 4 -jet NLO terms seems to destabilize the predictions. There are missing Sudakov terms needed to properly 'stitch' the different multiplicity samples together; it is hoped that the LoopSim technique may offer one way in supplying those missing terms.

Below in Figure 51, we show the NLO BlackHat+Sherpa predictions for the $H_{T}$ distribution for $W+\geq 2$ jets: the inclusive calculation to the left, the Exclusive Sums result adding $2+3$-jet NLO information in the middle and the Exclusive Sums result adding 2+3+4-jet NLO information to the right. Over the kinematic range covered in these plots, the Exclusive Sums technique adds less to the cross section at high $H_{T}$, although there is still a degradation of the scale dependence.


Fig. 50: The $W$ plus jets cross section, as a function of $H_{T}$, for $W+\geq 1$-jet production using the Exclusive Sums approach, and adding up to 3 jets at NLO (left) and 4 jets at NLO (right). The cross sections have been evaluated at a central scale of $H_{T} / 2$ and the uncertainty is given by varying the renormalization and factorization scales independently up and down by a factor of 2 , while ensuring that the ratio of the two scales is never larger than a factor of 2 .




Fig. 51: The $W$ plus jets cross section, as a function of $H_{T}$, for $W+\geq 2$-jet production using the inclusive NLO production (left) and the Exclusive Sums approach, adding up to 3 jets at NLO (center) and 4 jets at NLO (right). The cross sections have been evaluated at a central scale of $H_{T} / 2$ and the uncertainty is given by varying the renormalization and factorization scales independently up and down by a factor of 2 , while ensuring that the ratio of the two scales is never larger than a factor of 2 .

### 16.5 Towards interfacing BlackHat+Sherpa ntuples with LoopSim

LoopSim is a method to simulate higher order QCD corrections, in particular those beyond NLO. It is expected to work best for processes with large NLO-to-LO $K$-factor, however it was found to be advantageous even in some cases where the $K$-factor is moderate [437]. The method is based on unitarity and its main ingredient is a procedure that takes events from a process with $n+m$ partons in the final state and produces counter-term events with $n+m-1, n+m-2, \ldots, n$ particles, which approximate 1-loop, 2-loop, etc. contributions. In contrast to the Exclusive Sums method, it enables one to introduce (approximate) virtual corrections beyond 1-loop, thus ensuring that the $\alpha_{s} L^{2}$ type terms cancel for all the orders that are included. While we will not show LoopSim results that are directly comparable to the ATLAS data (the samples were generated before those cuts were made public), we will examine below the dependence on the $p_{t, \min }$ choice (which sets the size of $L=\ln O_{t} / p_{t, \min }$ where $O_{t}$ is a transverse observable) and see that it vanishes as $p_{t, \text { min }} \rightarrow 0$.

To distinguish between the exact result at the order $\mathrm{N}^{p} \mathrm{LO}$ and the result with simulated loops we use a notation in which we replace N by $\bar{n}$ for the orders simulated by LoopSim. So for example, $W+1$ jet at $\bar{n} \mathrm{LO}$ has approximate 1 -loop diagrams and is obtained by combining $W+1$ jet at LO with $W+2$ jet at LO where the latter is passed through LoopSim. Similarly $W+1$ jet at $\bar{n}$ NLO has exact 1-loop diagrams but simulated 2-loop contributions (by using $W+2$ jet at NLO as an input to LoopSim).

As argued in the previous section, the BlackHat+Sherpa ntuples allow one to efficiently perform a broad range of analyses. They have however a limitation. In order to reduce the size of stored files, the only partonic events that are recorded for the $W+n$-jet sample are those in which there are at least $n$ jets above a 20 GeV threshold. Since this threshold is below the jet cuts used by ATLAS and CMS, it is adequate for any NLO study of LHC jet cross sections. The situation is slightly more complex if we want to use the BlackHat+Sherpa ntuples to compute predictions beyond NLO using LoopSim. This is because the cut that is present in the $W+2$-jet BlackHat+Sherpa NLO sample eliminates part of the real contribution to the $W+1$-jet phase space at NNLO, for example $W+3$-parton events in which the 3 partons all form part of a single jet, or in which 2 partons form part of one jet, while the third is well separated in angle but below the 20 GeV jet threshold.

Since we plan to use LoopSim interfaced to BlackHat+Sherpa ntuples in our future study of multijet processes, it is important to directly check the effect of the finite generation $p_{t}$ cut, $p_{t, \mathrm{gen}}^{\min }$, on the predictions of the $p_{t}$ and $H_{T}$ distributions. We have performed such a study for $W^{-}+1$ jet generated with MCFM, where we varied a 'parton'- $p_{t}$ generation cut from 1 to $20 \mathrm{GeV}{ }^{32}$ This is not entirely equivalent to the cut in the BlackHat+Sherpa samples (which is applied to the standard jets, not to the partons), but should be adequate from the point of view of estimating the potential order of magnitude of finite generation cuts. The output from MCFM was interfaced to LoopSim which produced the additional loop diagrams. Then, the events were analyzed with the following set of cuts: $\left|y^{\text {lepton }}\right|<2.5, p_{T}^{\text {lepton }}>$ $20 \mathrm{GeV},\left|y^{\mathrm{jet}}\right|<4.5, p_{T}^{\text {jet }}>25 \mathrm{GeV}, m_{T, W}<20 \mathrm{GeV}$, where the anti- $k_{T}$ algorithm with $R=0.4$ was used for clustering.

The results are presented in Figure 52 where the ratios of cross sections obtained with a range of generation cuts are shown as functions of the $p_{t}$ of the leading jet and $H_{T, \text { jets }}$. At NLO, the only artefact we see is for the $p_{t, \text { gen }}^{\min }$ of 20 GeV in the bin below 40 GeV . This is as expected, since a 20 GeV cut on each of two partons can at most affect jets up to 40 GeV (such an artefact would not be present in the BlackHat+Sherpa samples). At $\bar{n} \mathrm{LO}$ and $\bar{n} \mathrm{NLO}$, however, the dependence on $p_{t, \mathrm{gen}}^{\min }$ is extended to a larger range of $p_{t, \text { lead.jet }} / H_{T, \text { jets }}$ and it is visible also for values of $p_{t, \text { gen }}^{\min }<20 \mathrm{GeV}$. However, even if the $p_{t, \text { gen }}^{\min }$ dependence of the $\bar{n} \mathrm{LO}$ and $\bar{n} \mathrm{NLO}$ results is stronger than at NLO, it dies out quickly with increasing $p_{t, \text { lead.jet }} / H_{T, \text { jets }}$ and becomes irrelevant at $\sim 100 \mathrm{GeV}$, depending on the observable and the

[^217]

Fig. 52: Ratios of cross sections from runs with a certain range of $p_{t, g e n}^{\min }$ values taken wrt. the cross section generated with $p_{t, \mathrm{gen}}^{\min }=1 \mathrm{GeV}$ for the distributions of $p_{t}$ of the leading jet (left) and the scalar sum of jets' transverse momenta, $H_{T, \text { jets }}$ (right).
order. This appears to be consistent with the expectation that the effect of the cut should vanish as a power of $p_{t, \text { gen }}^{\min } / p_{t, \text { lead.jet }}$ or $p_{t, \text { gen }}^{\min } / H_{T, \text { jets }}$.

Therefore we conclude, that in spite of the finite generation cut one should be able to trust the results obtained using BlackHat+Sherpa ntuples, above a moderate $p_{t}$ limit, even for more complex analyses such as those involving LoopSim.

### 16.6 Comparisons to data, Sherpa and HEJ predictions

In Figure 53 (left), we compare the ratio of the 2010 ATLAS $W$ plus jets data for the $H_{T}$ distribution for $W+\geq 1$ jets to predictions using the generic NLO calculation for $W+\geq 1$ jet, the Exclusive Sums approach adding up to 4 jets at NLO and the Monte Carlo event generator Sherpa. The agreement between the data and the pure NLO result is rather poor; it improves substantially with the inclusion of the Exclusive sums up to two jets at NLO, with further small improvements coming from higher multiplicities. As a reminder, we previously noted that the scale dependence improved when adding the 2 -jet NLO information, but degraded when adding higher jet multiplicities. The Sherpa prediction slightly overshoots the data for $H_{T}$ in the inclusive $W+1$-jet bin. We however note that the data versus Sherpa $H_{T}$ ratio has been formed based on the absolute normalization as given by the Monte Carlo simulation. Comparing the inclusive 1-jet cross sections, we find a factor of 0.97 between the data and the Sherpa result.

In Figure 53 (right), we compare the ratio of the 2010 ATLAS $W$ plus jets data for the $H_{T}$ distribution for $W+\geq 2$ jets to predictions using the generic NLO calculation for $W+\geq 2$ jet, the Exclusive Sums approach adding up to 4 jets at NLO, and to predictions from HEJ and from Sherpa. As noted previously, there is some increase in the predictions from the Exclusive Sums approach at the highest $H_{T}$ values, but not nearly as much as in the $W+\geq 1$-jet case. These increases go in the direction of closer agreement with the data, but the statistical error does not allow a clear judgement to be made. The Sherpa and HEJ predictions for this ratio are in reasonable agreement with the data but appear to fall off somewhat more rapidly at large $H_{T}$ than either the data or the various BlackHat+Sherpa predictions. Again this partly is the result of relying on the absolutely normalized Monte Carlo predictions, which yield $W+\geq 2$-jet normalization factors of 0.95 or 0.93 between data and Sherpa or HEJ, respectively.


Fig. 53: The ratios of the ATLAS $W+\geq 1$-jet (left) and $W+\geq 2$-jet (right) cross sections, as a function of $H_{T}$, taken wrt. various theory predictions. The absolute normalization has been kept as given by the calculations. The error bars represent the total fractional error (statistical plus systematic added in quadrature) at each point.


Fig. 54: (left) The fraction of the $H_{T}$ cross section for $W+\geq 1$-jet events arising from the $W+\geq 2$-jet, $W+\geq 3$-jet and $W+\geq 4$-jet final states derived from the Exclusive Sums approach, from Sherpa and from HEJ, compared to the 2010 ATLAS data. (right) The ratio of the cross sections for $W+\geq 3$ jets to $W+\geq 2$ jets, as a function of $H_{T}$, using predictions from the Exclusive Sums approach, from Sherpa and from HEJ, compared to the ratio from the 2010 ATLAS data.

In Figure 54 (left), we show the predictions for the fractions of the $H_{T}$ cross section in the inclusive $W+1$-jet bin arising from the inclusive $W+2$-jet, $W+3$-jet and $W+4$-jet final states as obtained from the Exclusive Sums approach and from Sherpa, compared to the 2010 ATLAS data. In Figure 54
(right), we show the ratio of the cross sections for $W+\geq 3$ jets to $W+\geq 2$ jets, as a function of $H_{T}$, again using predictions from the Exclusive Sums approach and from Sherpa but also from HEJ. We again compare to the ratio given by the 2010 ATLAS data. All three predictions agree with each other and with the data over the range considered, despite the big differences in the approaches. There may be an indication of some separation between the predictions at the very highest $H_{T}$ values.

### 16.7 Conclusions, outlook and future studies

The advances achieved over the last few years in calculating NLO corrections for multi-jet final states allow a more serious consideration of the possibility to combine various $n$-jet NLO predictions into an inclusive jet sample. The Exclusive Sums approach discussed in this contribution is a first promising step into this direction. More studies are required to understand the uncertainties related to this procedure. One way of doing so would be to test the stability of the predictions against variation of the jet algorithm and/or parameters of the jet algorithm used to obtain and separate the different NLO predictions for the fixed-multiplicity sets that eventually make up the sum of exclusive $n$-jet contributions. ${ }^{33}$

For the Exclusive Sums approach, outlined here for the case of $W+\geq 1$ jets, contributions are added proportional to $\alpha_{s}^{2}\left(W+1\right.$ jet at NLO), $\alpha_{s}^{3}$ ( $W+2$ jets at NLO), $\alpha_{s}^{4}(W+3$ jets at NLO) and $\alpha_{s}^{5}\left(W+4\right.$ jets at NLO), i.e. this procedure mixes powers of $\alpha_{s}$ and thus is missing essential Sudakov form factors that effectively bring each term to the same power of $\alpha_{s}$. One could imagine accomplishing this by embedding the NLO matrix elements in a parton shower Monte Carlo framework, however the technology for merging different multiplicities of NLO calculations with a parton shower is still under development. Note that at LO the tree-level matrix-element plus parton-shower merging methods (e.g. as implemented in Sherpa) are designed to satisfy this same- $\mathcal{O}\left(\alpha_{s}\right)$ requirement by including the (allorders) leading-log effects to the 'LO Exclusive Sums' exhibiting the LO analog of the Exclusive Sums discussed here. Compared to the matrix-element plus parton-shower merging, we see that the 'NLO Exclusive Sums' technique only accounts for Sudakov effects up to $\mathcal{O}\left(\alpha_{s}\right)$ while it describes each jet bin at full NLO instead of LO accuracy.

Relying on the parton shower Monte Carlo framework is not the only way to go in refining the Exclusive Sums strategy. Alternatively, the LoopSim method can be used to provide approximations to the higher-loop terms missing in the Exclusive Sums approach. As we have seen here, prospects for using it together with BlackHat+Sherpa ntuples seem promising. A detailed comparison of the LoopSim results to LHC data is however beyond the scope of this Les Houches contribution, though we look forward to it being carried out in the near future.

The ATLAS data taken in 2011 is about a factor of 130 times as large as the data taken in 2010 (the only published data for $W$ plus jets so far). This will allow a much further reach in all kinematic variables. To get an idea, we show in Figure 55 the ratio of the predictions from the Exclusive Sums to the respective inclusive NLO predictions for $W+\geq 1,2,3$ jets. At an $H_{T}$ value of 2 TeV , the ratio for $W \geq 1$ jet is of the order of 2 ; the ratio for $W \geq 2$ jets rises to about 1.4. The NLO-to-LO $K$ factor for $W+\geq 1$ jet rises rapidly with increasing $H_{T}$, while the $K$-factor for $W+\geq 2$ jets increases only moderately (because no new subprocesses are being introduced). It will be interesting to see if (a) the additional factor of 2 (for the $W+\geq 1$-jet case) and (b) the additional factor of approximately 1.4 (for the $W+\geq 2$ jet case) lead to better agreement with the data. The LHC data from 2011 (and the higher statistics expected in 2012) will reach these kinematic values and should shed further light on the necessity and the efficacy of this theoretical technique, not only for $W+\geq 1$ jet, but for higher jet multiplicities as well.

[^218]

Fig. 55: The ratio of the predictions obtained from the NLO Exclusive Sums approach to the inclusive NLO predictions for $W \geq 1$ jets, $W \geq 2$ jets and $W \geq 3$ jets. The ' jitter ' is due to the limited BlackHat+Sherpa statistics for these predictions.

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## Appendix: a double logarithmic analysis of the Exclusive Sums method

To help understand the structure of the Exclusive Sums method, it can be useful to consider how it works in a simple double logarithmic approximation. We use $p_{t, \min }$ to represent the minimum $p_{t}$ for the jets in the Exclusive Sums sample, and first study the cross section for $W$ production as a function of $p_{t, W}$ at high $p_{t, W}\left(\gg m_{W}\right)$, considering in particular the terms that go as $\alpha_{s}^{n} L^{2 n}$ where $L=\ln p_{t, W} / p_{t, \min }$. The 0 -jet sample does not contribute at all to non-zero $p_{t, W}$, so the first term comes from the exclusive 1 -jet contribution. If calculated to all orders in the double logarithmic approximation (DLA), it would have the form

$$
\begin{equation*}
\sigma_{1, \operatorname{excl}}^{\mathrm{DLA}}\left(p_{t, W}\right)=\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \exp \left(-\frac{2 C \alpha_{s}}{\pi} L^{2}\right) \tag{100}
\end{equation*}
$$

where $C=2 C_{F}+C_{A}$ for the (dominant) $q g \rightarrow W^{ \pm} q^{\prime}$ scattering process. The $n$ exclusive jet rate would be given by

$$
\begin{equation*}
\sigma_{n, \mathrm{excl}}^{\mathrm{DLA}}\left(p_{t, W}\right)=\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \frac{1}{(n-1)!}\left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)^{n-1} \exp \left(-\frac{2 C \alpha_{s}}{\pi} L^{2}\right) \tag{101}
\end{equation*}
$$

and one sees that the sum over all multiplicities is given by

$$
\begin{equation*}
\sigma\left(p_{t, W}\right)^{\mathrm{DLA}}=\sum_{n=1}^{\infty} \sigma_{n, \mathrm{excl}}^{\mathrm{DLA}}\left(p_{t, W}\right)=\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \tag{102}
\end{equation*}
$$

i.e. in the double logarithmic approximation, there are no corrections to the $p_{t, W}$ distribution at high $p_{t, W}$. Now let us consider what happens if we expand each of the exclusive sums to NLO. For the $n$-jet cross section, we have

$$
\begin{equation*}
\sigma_{n, \mathrm{excl}}^{\mathrm{NLO}(\mathrm{DLA})}\left(p_{t, W}\right) \simeq \sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \frac{1}{(n-1)!}\left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)^{n-1}\left(1-\frac{2 C \alpha_{s}}{\pi} L^{2}\right) \tag{103}
\end{equation*}
$$

Performing the sum over $n$, which corresponds to summing an infinite tower of NLO exclusive jet calculations, leads to

$$
\begin{align*}
\sigma\left(p_{t, W}\right)^{\mathrm{DLA}} & =\sum_{n=1}^{\infty} \sigma_{n, \mathrm{excl}}^{\mathrm{NLO}(\mathrm{DLA})}\left(p_{t, W}\right)  \tag{104a}\\
& =\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right) \exp \left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)\left(1-\frac{2 C \alpha_{s}}{\pi} L^{2}\right)  \tag{104b}\\
& =\sigma_{1}^{\mathrm{LO}}\left(p_{t, W}\right)\left(1-\frac{1}{2}\left(\frac{2 C \alpha_{s}}{\pi} L^{2}\right)^{2}+\mathcal{O}\left(\alpha_{s}^{3} L^{6}\right)\right) . \tag{104c}
\end{align*}
$$

As long as $L^{2}$ is not large, the difference between this and the correct answer of Eq. 102 is a straightforward NNLO correction, i.e. small. However when $p_{t, W} \gg p_{t, \min }$ the logarithms become large, the $\alpha_{s}^{2} L^{4}$ term can be of order 1 and the Exclusive Sums method may then no longer be a good approximation. A similar analysis can be performed for an exclusive sum truncated at some finite order, as used in our study.

Given the above discussion, one may wonder then if there are any circumstances in which the Exclusive Sums method will bring benefits. For the observable studied in this contribution, $H_{T}$, the key difference with respect to $p_{t, W}$ is that it is subject to a 'giant' $K$-factor at NLO. This phenomenon is associated with 'dijet' topologies in which a soft or collinear $W$ is radiated off the dijet system, leading to a double logarithmic (electroweak) enhancement. In addition these topologies can be created by $q q$ type scattering (whereas the LO process involves only $g q$ or $q \bar{q}^{\prime}$ scattering), leading to further enhancement in $p p$ collisions at large $H_{T}$. Dijet type topologies contribute significantly to the $H_{T}$ distribution, even when the $W$ is soft, because the variable sums all particles' transverse momenta (whereas the softness of the $W$ limits these topologies' contribution to the $p_{t, W}$ distribution).

Because of the giant $K$-factor, for the $H_{T}$ variable the behaviour of the Exclusive Sums method is more subtle than for $p_{t, W}$ : while the $\sigma_{W+2}^{\mathrm{NLO}}$ contributions destabilize the prediction for the $q g \rightarrow W q^{\prime}$ type topologies, they instead stabilize the prediction for the much larger $q q \rightarrow W q^{\prime} q$ topologies (present only at LO in a NLO $W+1$-jet calculation). Going further in the exclusive sum, however, i.e. including $\sigma_{W+3}^{\mathrm{NLO}}$ and $\sigma_{W+4}^{\mathrm{NLO}}$ contributions can however destabilize the predictions for both kinds of topologies. Traces of this behaviour were visible in the numerical studies shown above.

## 17. $W$ PRODUCTION IN ASSOCIATION WITH MULTIPLE JETS AT THE LHC ${ }^{34}$


#### Abstract

We compare the results from four different theoretical predictions for the production of a $W$ boson in association with at least two jets at the Large Hadron Collider. We discuss a possible method for combining next-to-leading order samples with different jet multiplicity from BlackHAT+SHERPA. We then compare these results with the next-to-leading order $W$ plus two jet calculation, the leading order ME\&TS merged approach of SHERPA and the highenergy resummation approach of High EnERGY JETS in an attempt to determine if these approaches can be distinguished at the LHC.


### 17.1 INTRODUCTION

The production of a $W$ boson in association with jets at the Large Hadron Collider (LHC) is an extremely important process. It contributes to three distinct areas of the rich physics program at the LHC. Firstly, it is a key Standard Model signal and therefore important to test our understanding of the Standard Model in the TeV -scale energy range. Secondly, it is an important background in many searches for new physics where, for example, new heavy coloured particles have cascade decay chains. Thirdly, it provides an ideal testing ground for experimental techniques such as a jet veto: what is learned in the relatively well-understood treatment of $W$ plus jets can be directly applied to Higgs searches for example.

It has been observed that the ratio of $W+(n+1)$-jet events to $W+n$-jet events can be substantially larger than one might naïvely expect by considering the $\alpha_{s}$ suppression only. This is especially true in phase-space regions of large four-momenta, such as the high- $H_{T}$ tail, because the available phase space for extra jet emission at the LHC is extremely large. It can therefore compensate for the effect of an additional factor of the strong coupling. This effect is more visible in distributions where additional radiation leads to a significant change in the value of the observable, as is the case for the $H_{T}$ distribution, the scalar sum of the transverse momenta of identified leptons, jets and missing energy. The change will be more moderate in an observable like $H_{T, 2}$, whose definition differs from that of $H_{T}$ by truncating the jet sum to include only the two hardest jets in the event. To make an impact here requires the radiation to lead to an additional jet with transverse momentum as large as that of the second hardest jet, not only larger than the jet $p_{T}$ threshold. The effects will also be smaller in more inclusive variables like the transverse momentum of the $W$ boson, $p_{T, W}$, or the leading jet, $p_{T, j_{1}}$.

There are a number of different theoretical approaches to describing the emission of large numbers of jets. In order to probe to what extent the differences in these will be accessible at the LHC, we will compare, in this study, the predictions for the jet activity in inclusive $W(\rightarrow e \nu)+2$-jet production from (a) BLACKHAT+SHERPA $(B H S)$ [70, 51, 22], (b) combined $B H S$ samples (to be described below), (c) Sherpa [146, 425] run in ME\&TS mode (S-MEPS) [426, 427, 428] and (d) High Energy Jets (HEJ), an all-order resummation of wide-angle radiation [418, 419, 438].

The current state-of-the-art next-to-leading order (NLO) predictions for $W$ production in association with jets are those of $B H S$, which have been calculated up to $W$ plus four jets with a leading-colour approximation for the virtual part [22], and up to $W$ plus three jets with a full color treatment [70, 51]. In this study, we consider the inclusive $W+2$-jet prediction at NLO accuracy, and further, discuss and show predictions from an inclusive sample where $W+2,3,4$-jet events generated by $B H S$ are combined in a simple manner, nevertheless without introducing any double counting of phase-space regions.

The $S$-MEPS predictions are obtained from merging at leading order (LO) tree-level Matrix Elements for $W+0, \ldots, n$-parton final states with (Truncated) parton Showers (hence the name ME\&TS) preserving the leading logarithmic accuracy to which soft and collinear multiple emissions are described by the parton shower. The newer ME\&TS merging scheme was introduced in Ref. [426] and optimised

[^219]as documented in Refs. [427, 428] to improve over the original SHERPA implementation based on the CKKW approach [429, 430]. ME\&TS guarantees a better matching regarding the usage of scales as occurring in the evaluation of the matrix elements and those scales driving parton showering. The $S$-MEPS sample used in our study was generated by including $W(\rightarrow e \nu)$ production matrix elements with up to five extra partons (massless quarks, $u, d, s, c, b$, and gluons).

The HEJ framework is a resummation of the leading logarithmic terms occurrung in pure, or $W$, $Z$ or $H$ plus, multi-jet production in the limit of large invariant mass between each pair of jets, to all orders in $\alpha_{s}$. This is then matched to tree-level accuracy for final states with two, three or four jets. In principle, the HEJ framework can be merged with a parton shower to add the collinear pieces which are not included in the HEJ description (HEJ does include soft emissions down to around 2 GeV ). First steps in this direction for pure jet production were taken in [431]. Here, the HEJ predictions are calculated at the parton level.

In the 17.2 section, we will elaborate on the method (b) for combining NLO samples of different jet multiplicities. Then, in the 17.3 section, we will first show explicit results of the sizable impact of large multiplicity events by comparing predictions from the combined BHS sample and the S-MEPS merged sample. Secondly, we will study variables chosen to probe the differences in the treatment of the QCD radiation. We will show and compare the predictions for all four descriptions mentioned above focusing on the following observables:

- the average number of jets as a function of $H_{T}=\sum_{i} p_{T, j_{i}}+p_{T, e}+p_{T, \nu}$ and $\Delta y$, the rapidity difference between the most forward and most backward jets, and also
- the ratio of the inclusive 3-jet rate to the inclusive 2-jet rate as a function of $H_{T}$ and $\Delta y 35$

We will then discuss the areas of agreement and difference that we find, before we finally conclude in the 17.4 section.

### 17.2 NLO EXCLUSIVE SUMS

An NLO $n$-jet prediction contains events with $n$ or $n+1$ partons. For observables for which higher multiplicites have a significant impact, this limitation can be detrimental. If one has predictions for different multiplicities ( $m, m+1, \ldots, M$ ), one can try to combine them by avoiding double counting by requiring that the $n$-jet prediction is used only to describe $n$-jet events (except for the highest multiplicity where ( $n+1$ )-jets configurations are allowed). The total cross section can be rewritten as a decomposition based on exclusive (exc) and inclusive (inc) jet bins:

$$
\begin{equation*}
\sigma^{\mathrm{tot}} \equiv \sigma_{m}^{\mathrm{inc}}=\sum_{n=m}^{M-1} \sigma_{n}^{\mathrm{exc}}+\sigma_{M}^{\mathrm{inc}} \tag{105}
\end{equation*}
$$

The exclusive-sums procedure describes each jet bin at NLO accuracy, i.e. at $\mathcal{O}\left(\alpha_{s}^{n+1}\right)$, or, alternatively, only the $(M+1)$-th (inclusive) jet bin is predicted with LO precision. We hence note that the combination of the terms shown in Eq. 105) occurs at different orders of the strong coupling. Furthermore, the definition of an exclusive $n$-jet sample requires a detailed treatment of jet vetoing. For these reasons, the simple combination procedure is crude and does not increase the formal accuracy of the prediction, which is that of NLO of the smallest multiplicity. However, one can hope that the procedure will lead to a better prediction in observables where higher multiplicity events dominate.

More studies are required to understand the uncertainties related to this procedure. One way of doing so would be to vary the jet algorithm and/or parameters of the jet algorithm used to separate the different NLO predictions into fixed multiplicities sets and test the stability of the prediction ${ }^{36}$ This is left to a future study.

[^220]\[

$$
\begin{array}{ll}
\left|\eta_{e}\right|<2.5 & p_{T, e}>20 \mathrm{GeV} \\
M_{\perp, W}>20 \mathrm{GeV} & p_{T, \nu}>20 \mathrm{GeV} \\
\left|\eta_{j}\right|<4.5 & p_{T, j}>25 \mathrm{GeV}
\end{array}
$$
\]

Table 12: Summary of the cuts applied in the analysis.


Fig. 56: The average number of jets as a function of $p_{T, W}$ (left) and $p_{T, j_{1}}$ (right). The $p_{T, W}$ plot shows the $B H S$ exclusive sums prediction, while the $p_{T, j_{1}}$ plot is obtained from $S$-MEPS.

### 17.3 RESULTS OF THE COMPARISON

In this section, we compare the results of different theoretical descriptions for $W+n$-jets production at the LHC. The number $n$ can take values from 2 and above, as we will mostly consider inclusive samples. The four descriptions, which we will compare here in more detail, are

- the $B H S$ calculation of $W+2$-jets at NLO,
- the combined sample of $W+2,3,4$-jet events at NLO from $B H S$, as described in the 17.2 section,
- the $S$-MEPS merged $W+n$-jets sample using LO tree-level matrix elements up to $n=5$, and
- the approach of HEJ.

Throughout this study, we will consider inclusive samples of $W^{-}$boson production in association with at least two hard jets identified by the anti- $k_{T}$ jet algorithm using $R=0.4$. The jets are required to have $p_{T, j}>25 \mathrm{GeV}$. We look only in the $W^{-} \rightarrow e^{-} \bar{\nu}_{e}$ decay channel and use the cuts given in Tab. 12 where $M_{\perp, W}$ is defined as $M_{\perp, W}=\sqrt{\left(\left|\vec{p}_{T, e}\right|+\left|\vec{p}_{T, \nu}\right|\right)^{2}-\left(\vec{p}_{T, e}+\vec{p}_{T, \nu}\right)^{2}}$.

The HEJ predictions use the geometric mean of the jet transverse momenta to determine the renormalisation and factorisation scale, i.e. $\left(\prod p_{T, j}\right)^{1 / n}$. This central choice will be varied by a factor of two in either direction to provide an envelope (marked by dotted lines in the corresponding figures) around the HEJ default prediction. The BHS predictions instead use $\hat{H}_{T}^{\prime} / 2$ as the NLO calculation becomes unstable for a scale which is too low. In the $S$-MEPS calculation, scales are chosen according to the default prescription given by ME\&TS [426].

The variables $H_{T, 2}, p_{T, W}$ and $p_{T, j_{1}}$ are less sensitive to the presence of additional radiation than $H_{T}$, as discussed in the introduction. The plots, which we present in Figs. 56 and 57 address the alternative question: given a particular value of $H_{T}, H_{T, 2}$ etc. how many jets are typically found in the event?

Figs. 56 and 57 show the stacked results for the average number of jets as a function of $p_{T, W}, p_{T, j_{1}}$, $H_{T}$ and $H_{T, 2}$ visualising the contributions from each exclusive 2,3,4-jet sample and the inclusive 5 -jet


Fig. 57: The contribution from different multiplicities to the average number of jets as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the BHS exclusive sums prediction, while the lower ones are extracted from S-MEPS.
sample. The left (right) plot in Fig. 56 and the upper (lower) rows of plots in Fig. 57 depict the results as obtained from the combined BHS sample (the $S$-MEPS sample). In all cases the different colours correspond to the terms in the numerator of the formula for the average number of jets,

$$
\begin{equation*}
\langle N\rangle_{5}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{106}
\end{equation*}
$$

where blue, green, red and magenta stand for $i=2,3,4$ and $i=5$, respectively. The subscript to $\langle N\rangle$ clarifies that we truncate the determination of the average after the fifth jet bin, noting that $\langle N\rangle_{k} \rightarrow\langle N\rangle$ for a sufficiently large number of jet bins. This makes no difference for the BHS predictions employed here since the jet multiplicity de facto is limited to five, but it does for the $S$-MEPS and HEJ computations where events with $i>5$ jets do occur. We have defined $n_{k}^{\text {exc } / \mathrm{inc}}=d \sigma_{k}^{\text {exc } / \mathrm{inc}} / d O$ where $O$ denotes an observable like $H_{T}$, or $\Delta y$ presented later on. Note that in Fig. 57 the 5 -jet part contributes to the average number of jets with a factor of 5 , while the 2 -jet part, for example, contributes with a factor of 2 only.

The layout of Fig. 58 (including the colour coding) is the same as before: here, we however display, wrt. $n_{2}^{\text {inc }}$, the relative fractions of the different multiplicities corresponding to the terms in the denominator of Eq. (106). In other words, in Fig. 58 we consider the partitioning of

$$
\begin{equation*}
1=\frac{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{107}
\end{equation*}
$$



Fig. 58: The fraction of the total rate from different multiplicities as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the $B H S$ exclusive sums prediction, while the lower ones are extracted from $S$-MEPS.

Although there is just a $30 \%$ fraction of inclusive 5 -jet events to the total cross section, we observe that their contribution to the build-up of $\langle N\rangle\left(H_{T}\right)$ for very large $H_{T}$ gets close to $50 \%$. Also, for an $H_{T} \sim$ 500 GeV , the average number of jets is composed evenly between the 2,3 -jet and 4,5 -jet contributions, while the relative fraction of the 2,3 -jet events is nearly $70 \%$. This emphasizes the dominance of multijet events in forming large $H_{T}$ values. It also can be seen that for medium $H_{T}$ values, $400<H_{T}<$ 700 GeV , all the multiplicities give roughly the same contribution to the variable $\langle N\rangle\left(H_{T}\right)$, while for low $H_{T}$, the average is primarily described by 2-jet events.

Going clockwise through Figs. 56 and 57 we see that the average number of jets is indeed sensitive to higher multiplicities when considered as a function of $p_{T, W}, p_{T, j_{1}}$ and $H_{T, 2}$, but in all these cases this happens to a lesser extent as if considered as a function of $H_{T}$. As expected, the dependence is mildest for $p_{T, W}$, the most inclusive observable studied here. We also observe that the jet-bin decomposition of $p_{T, j_{1}}$ and $H_{T, 2}$ turns out very similar. Most strikingly we note the increase in the contribution from the highest multiplicity events, the ones containing more or at least five jets. For $H_{T, 2}$, we furthermore display to the right of Fig. 58 the relative fractions as done in the $H_{T}$ case. Even for largest $H_{T, 2}$ values, the fraction arising from 2,3 -jet events remains close to $65 \%$ stressing once more the lower sensitivity of $H_{T, 2}$ versus $H_{T}$ regarding multiple jet production.

Finally, we compare the plots from the combined BHS samples in all figures to the corresponding ones generated with the $S$-MEPS sample. Interestingly, the outcome looks very similar although ME\&TS handles the single terms in Eq. (105) rather differently. They are calculated at least at leading (soft/collinear) logarithmic accuracy improved by LO $n$-jet effects. Presumably, for the exclusive jet bins, this description (which allows a better treatment of jet vetoes) is not too far off the exclusive sums


Fig. 59: Average number of jets as a function of $H_{T}$ (left) and $\Delta y$ (right) in two BHS descriptions, from $H E J$ and from $S$-MEPS, the latter using the $\langle N\rangle_{7}$ definition. The bands shown with dotted lines for the HEJ prediction are a result of varying the scale by a factor of 2 in each direction.
approach, since the unresolved $\mathcal{O}\left(\alpha_{s}\right)$ corrections are also present in the Sudakov form factors applied in the ME\&TS approach. Also, the combined BHS samples as well as the $S$-MEPS sample use the same tree-level matrix elements, namely up to $W+5$-parton matrix elements. Clearly, it has to be studied further whether this similarity in the results is a coincidence or not.

It is clear that the impact of the higher multiplicity samples is significant throughout, especially in the high $H_{T}$ tail. This is precisely the region, which would be probed for signs of new physics, and therefore it is essential that we fully understand our theoretical descriptions in this region. This is the subject of the remainder of this contribution, where we compare all four different methods of modelling hard QCD radiation in inclusive $W+2$-jet events.

The left plot of Fig. 59 shows the final comparison plot between the exclusive sums and inclusive 2-jet $B H S$ results as well as the $H E J$ and $S-M E P S$ predictions for the average number of jets as a function of $H_{T}$. The differences in the descriptions are significantly larger than the scale uncertainty band on the $H E J$ prediction. For the $W+2$-jet NLO result, the number of jets rises to 2.6 already at $H_{T}=500 \mathrm{GeV}$ but that levels off significantly below the $S-M E P S$, exclusive $B H S$ sum and $H E J$ results. The $H E J$ results level off at a higher value of about 3.0 , starting to clearly disagree with the exclusive sums and $S$-MEPS predictions above 500 GeV , from where those two curves keep rising to a final level of around 3.7 to 4.0. The $S$-MEPS comes in highest at largest $H_{T}$, where $\langle N\rangle_{7}$ is shown, cf. Eq. (106), in order to determine the average number of jets for this $S$-MEPS result. The reason for giving slightly higher $\langle N\rangle$ than the exclusive sums lies in the contribution of additional parton-shower jets present in the $S$-MEPS calculation and more accurately accounted for by the use of the $\langle N\rangle_{7}$ definition as compared to the earlier result based on $\langle N\rangle_{5}$ presented in Fig. 57 to the lower left.

In the right panel of Fig. 59, we have plotted the average number of jets as a function of the rapidity span, $\Delta y$, instead of $H_{T}$ as before. Again the differences are larger than the scale variation shown on the HEJ result, but the ordering is different to that of the left plot of Fig. 59. All four descriptions increase linearly with $\Delta y$ but the gradient is steepest for the HEJ predictions where the average rises above 3.0 for $\Delta y$ values as large as 6.0. The BHS exclusive sum result is consistently below this, reaching about 2.8 at $\Delta y=6.0$, and agrees pretty well with the $S$-MEPS result based on $\langle N\rangle_{7}$. The NLO $W+2$-jet prediction given by $B H S$ is lower still, between 2.4 and 2.5 for $\Delta y \sim 5.0$.

It may seem surprising that on the plot on the left-hand side the exclusive sums and S-MEPS lie higher for most of the distribution whereas on the right-hand side these approaches as well as $H E J$ give predicitions that are commensurate. The region of high $H_{T}$ and that of high $\Delta y$ however are largely distinct as it is very expensive to have both a large rapidity and large $p_{T}$ for the jets. Also while radiating


Fig. 60: The ratio of the inclusive 3 -jet and 2 -jet rates in the inclusive $W+2$-jet NLO and exclusive sum description of $B H S$ as well as in the $S$-MEPS and $H E J$ approaches as a function of $H_{T}$ (left) and $\Delta y$ (right). Again, the dotted lines indicate the uncertainty band from varying the scale in $H E J$ by a factor of 2 in each direction.
an additional jet automatically moves an event towards the higher $H_{T}$ direction, radiating an additional jet tends to not change the rapidity difference. So, we expect the higher multiplicies to have a smaller effect on the average number of jets as a function of $\Delta y$ compared to as a function of $H_{T}$. This is indeed the case in Fig. 59.

Lastly, in Fig. 60 we plot the ratio of the inclusive 3 -jet to the inclusive 2 -jet rate as a function of $H_{T}$ (left) and $\Delta y$ (right), again for all four descriptions used here. The predicted $\left(d \sigma_{3}^{\text {inc }} / d H_{T}\right) /\left(d \sigma_{2}^{\text {inc }} / d H_{T}\right)$ all agree very well below 400 GeV . The fixed order $B H S$ result for $W+2$ jets is highest for large $H_{T}$, however is known to become unreliable here, since the probability that an inclusive 2 -jet event is at least a 3 -jet event turns too large, being in conflict with the expected behaviour of an $\mathcal{O}\left(\alpha_{s}\right)$ correction. The BHS exclusive sums, the S-MEPS and the HEJ results, in this order, level off considerably lower with the HEJ fraction staying below $60 \%$ to $70 \%$, which leaves the other predictions again above the $H E J$ uncertainty envelope. In contrast, when the same ratio of jet rates is plotted against $\Delta y$, the $H E J$ prediction is consistently higher throughout. This again emphasises that differences in the descriptions come to light in different kinematic regions. However, in both cases here the magnitude of the differences is relatively small and would be rather difficult to distinguish in present experimental data.

### 17.4 CONCLUSIONS

We have compared a number of theoretical descriptions of $W^{-}$production in association with at least two jets. After outlining one possible method of combining NLO calculations of different multiplicities, we compared this with a pure NLO calculation of $W+2$-jets production obtained by BLACKHAT+SHERPA, a sample of leading-order events merged using the ME\&TS method of SHERPA, and the high-energy resummation of the HEJ framework.

We studied the average number of jets and the ratio of the 3 -jet and 2 -jet inclusive cross sections as a function of $\Delta y$ and of $H_{T}$. We find, with these simple cuts, some clear differences in the predictions when we study the average number of jets as a function of both $\Delta y$ and $H_{T}$. Smaller differences, which would be more difficult to disentangle experimentally, are found when we study the ratio of inclusive rates.

It would be very valuable to have an experimental study, which probed the average number of jets in $W$ production in association with at least two jets, to test our different descriptions of these important Standard Model processes.

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## 18. UNCERTAINTIES IN THE SIMULATION OF $W+$ JETS - A CASE STUDY 37


#### Abstract

In this contribution, uncertainties in the simulation of a large variety of observables related to the production of $W$ in association with jets at the LHC and the Tevatron are discussed. This work aims to - serve as a compendium of currently publicly accessible tools in addition to the ones presented in a previous publication [439] with a similar topic, and to compare their results; - discuss the origin and generic size of various uncertainties in the simulation of perturbative and non-perturbative aspects of this process; - trace the interplay of these uncertainties in various stages of the full event simulation; - hint at those uncertainties in each of the various tools considered here which the respective authors find relevant; - guide their users in how to assess the related uncertainties in a way the authors recommend.


### 18.1 Introduction

The production of $W$-bosons in association with jets constitutes an important process at the Tevatron and the LHC, for a variety of reasons. First of all, it represents a major background to Standard Model signatures such as top-pair and single-top production, and it also plays a role in searches for the Higgs boson in the Standard Model. Furthermore, this reaction, together with the fairly similar channel of $Z$ production in association with jets, provides one of the most important backgrounds in those searches for new physics where large missing transverse energy and high jet multiplicities characterise the respective signal. Thirdly, this process has become a standard reaction for QCD studies at hadron colliders, ranging from the validation of simulation tools for multijet signatures to measurements related to multiple parton scattering. Finally, this process also provides one of the main testbeds for novel techniques in the automation of higher-order QCD corrections and their matching or merging with subsequent parton showers in the framework of event generators.

In the spirit of this last point, providing a testbed for the combination of fixed order calculations with the parton shower, this process has been analysed in quite some depth in [439] about five years ago. A number of reasons provide motivation to update and extend this previous study, namely

- the LHC being up and running and starting to provide highly precise data such that a proper treatment of uncertainties becomes an important issue;
- major improvements in the ability to calculate higher-order corrections including up to four jets in the final state accompanying the $W$ bosons [51, 117, 22];
- the advent of such next-to leading order calculations - albeit for lower final state multiplicities fully matched to the parton shower [440, 404, 424];
- an improved understanding of the leading order merging prescription for towers of multijet multiplicities with the parton shower [426, 441];

[^221]- the combination of matching and merging methods [442, 443];
- and new methods to simulate multijet topologies based on the high-energy limit [64].

Therefore this study aims at being a first step towards a more complete update of [439], with a shift in focus towards a discussion of theoretical uncertainties in different approximations, including perturbative and non-perturbative effects. Apart from tracing the origin and determining the generic size of various uncertainties in the theoretical description of various observables related to this process, also the interplay of them at various stages of the simulation, from the matrix element to the hadron level will be discussed. Consequently, the most important causes for theory uncertainties in various tools are highlighted. Therefore, one of the more practically relevant goals is to also provide methods to reliably and robustly estimate such uncertainties for the various tools used in this study, as recommended by authors or users.

The outline is as follows: After briefly presenting the various tools included in this study and discussing the way they have been used here in Sec. 18.2 , example results for them will be presented individually, tool by tool in Sec. 18.3 . In Sec. 18.4 these results are compared in order to see and quantify relative differences. In this endeavour, experimental results have not yet been included. We reserve this comparison with relevant data for a later, full-fledged analysis, which will hopefully include even more tools.

### 18.2 Codes

In this work a variety of different codes has been employed, which allow to study the process at various different stages:

1. Fixed order matrix elements:

By now, the description of $W$ boson production in association with jets is possible for up to 4 additional jets at NLO. Here, results from two NLO codes, GoSAM+SHERPA [12, 425, 146] and BLACKHAT+SHERPA [70, 51, 22], which are either publicly available or provide publicly available event files, are presented. The corresponding results therefore are on the matrix element level.
2. All-order resummed matrix elements:

Approximations to the partonic matrix elements for the processes of $n$-jet production, and $W, Z, H+n$-jets, $n \geq 2$, was recently calculated to any multiplicity, and including all-order resummations for the leading virtual corrections. The all-order scheme [418, 419], implemented in the HEJ [64] code, becomes exact in the limit of large invariant mass between each parton (the MRK limit of BFKL). The resummation scheme is merged with LO matrix elements (much like in MEPS, see later). The resummation of HEJ can also be interfaced to a parton shower [431]; the results presented here, however, are on the matrix element level. It should also be stressed that due to the nature of the approximation of HEJ, the simulation here are relevant for the production of at least two jets in addition to the $W$ boson.
3. Parton showers:

The pure parton shower code relies on the collinear approximation to produce additional jets. By using a matrix element reweighting, however, in the process of $W$ production, typically one additional jet can correctly be described. For this simulation, PYTHIA8 [348] has been used here, with results available on the parton shower level, hadron level and hadron level including UE.
4. LO matrix elements merged with the parton shower (MEPS):

By now, the use of towers of multijet matrix elements with increasing multiplicity merged to the parton shower following ideas presented in [444, 429, 445, 430] is common practise in the experimental collaborations. In fact, a first comparison of different codes and implementation has been presented a while ago [439]. Here, three implementations of these ideas are included, namely the ones in MADGRAPH+PYTHIA [165, 446, 163, 191, 400], PYTHIA8+ME [441] and SHERPA [146]. Here results are available on all levels matrix element level, parton shower level, hadron level,
hadron level including UE, and hadron level including UE and QED final state radiation in different combinations of codes.
5. NLO matrix elements matched to the parton shower ( $\mathrm{NLO} \otimes \mathrm{PS}$ and MENLOPS):

In principle two methods by now have been proposed and fully implemented which consistently match full NLO calculations to the parton shower, namely Mc@NLO [401] and Powheg [416, 417]. Here the latter is being used, with its implementation in the Powheg Box [13], and interfaced to the PYthia [400] parton shower in its $k_{T}$-ordered version [447]. In addition, a combination of such matching with the merging methods described in the previous point is available [442, 443], ranging under the name MENLOPS. In this paper we use an implementation of such methods provided in the SHERPA framework. In both cases, results are available on all levels matrix element level, parton shower level, hadron level, and hadron level including UE.

### 18.21 BLACKHAT + SHERPA

The NLO predictions are obtained by combining BLACKHAT [4] for the virtual part and SHERPA [147, 448] for the real part. It is currently possible to obtain predictions at NLO for a $W$-boson in combination with up to four jets [70, 51, 22].

The plots have been produced by re-analysing large event files produced by the combination of BLACKHAT and SHERPA. These files contain particle four-momenta as well as the coefficients of all scale dependent functions, including the PDFs so that it makes it possible to easily change factorisation and renormalisation scales as well as the PDF set.

We used a common factorisation and renormalisation scale $\mu_{F}=\mu_{R}=\hat{H}_{T}^{\prime} / 2$ with $\hat{H}_{T}^{\prime}=$ $\sum_{j} p_{T}^{j}+E_{T}^{W}$ where the sum runs over all jets and $E_{T}^{W}=\sqrt{M_{W}^{2}+\left(p_{T}^{W}\right)^{2}}$.

Estimation of uncertainties The estimation of the uncertainties for the NLO calculation obtained with BLACKHAT+SHERPA is obtained by combining in quadrature the pdf uncertainties obtained using the pdf error set and the uncertainties obtained by varying the factorisation and renormalisation scales simultaneously by factors of $1 / 2$ and 2 . To this error we also add in quadrature the integration error estimate. Another way of estimating the uncertainties due to the choice of scales is to compare predictions obtained using different choice of basis scales, but this has not been done for this study.

We used the CTEQ6.6 PDF set. The value of $\alpha_{s}$ used for this calculation has also been taken as that provided with this PDF set. The PDF uncertainties are estimated using the hessian method and PDF 'error' set provided with the CTEQ6.6 PDF set.

### 18.22 GOSAM + SHERPA

GOSAM [12] is a new framework which allows the automated computation of one-loop scattering amplitudes for multi-particle processes. The one-loop scattering amplitudes are generated in terms of algebraic $d$-dimensional unintegrated amplitudes, which are obtained via Feynman diagrams. This allows to perform symbolic manipulations of the expressions prior any numerical step. For the reduction, the program offers the possibility to use either a $d$-dimensional extension of the OPP method [121, 122, 119], as implemented in SAMURAI [6], or tensor reduction as implemented in golem95 [130, 131] interfaced through tensorial reconstruction at the integrand level [124].

The GoSAM framework can be used to calculate one-loop corrections within both QCD and electroweak theory. Beyond the Standard Model theories can be interfaced using FeynRules [137] or LanHEP [136].

To produce results for a certain process specified by the user, the program must be fed with an "input card" with the details of the process. Alternatively, when interfacing the program with a Monte

Carlo (MC) event generator which supports the Binoth-Les-Houches-Accord (BLHA) interface [145], the specific order file produced by the MC event generator can be passed to GoSAM.

The analysis presented here was performed using this latter generation mode and SHERPA [425] 146] was chosen as MC event generator. SHERPA provides therefore the matrix elements for the production of $W$ and exactly one jet at the Born-level and the NLO real corrections to it, together with the needed subtraction terms and their integrated counter-parts. GOSAM provides the NLO virtual-part. The generation of the code follows the standards of the BLHA-interface [145]. During the first call of Sherpa an "order file" is written by the MC program. This file is read-in by GOSAM to produce the code for the one-loop evaluation of needed process. If this happens successfully, a contract file with information on the different possible subprocesses is produced by GoSAM and can be later read by the MC generator to recognize the numbering of the different partonic subprocesses. At running time all information between GoSAM and SHERPA is also passed using the BLHA-interface standards.

The steering of the event generation and the analysis interface with RIVET [360] is done using SHERPA cards. Each curve in the analysis consists of 100 combined runs of 50 million events. The renormalisation and factorisation scales are set according to the choice made for this analysis in Les Houches to

$$
\mu_{F}=\mu_{R}=\hat{H}_{T}^{\prime} / 2
$$

where $\hat{H}_{T}^{\prime}$ is defined in the previous section.

Estimate of uncertainties The estimation of the uncertainties for the NLO calculation obtained with GoSAM+SHERPA is done combining in quadrature the PDF uncertainties with the uncertainty coming from the separate variation of factorisation and renormalisation scale by factors of $1 / 2$ and 2 . Ideally also the integration error should be added in quadrature to the previous estimate, however the MC integration error obtained with RIVET at NLO is not reliable because of the incapacity of RIVET to take into account properly the correlation between real and subtraction events. For this reason and because of the very high statistics of the MC sample, the MC integration error is neglected. To assess the PDF uncertainty we compute the envelope of the results obtained using the three different PDF sets CT10 [255], used as nominal set, MSTW08 [262] and NNPDF2.1 [312]. The total scale uncertainty is determined by adding in quadrature the factorisation and renormalisation scale uncertainties. Each of them is found by computing the maximum between the nominal value and the up and down variations.

### 18.23 HEJ

The High Energy Jets (HEJ) framework [418, 419] provides an alternative description of collider events to the standard fixed order calculations (possibly interfaced to a parton shower). Instead, HEJ uses approximations to the hard scattering matrix element to all orders in $\alpha_{s}$ which become exact in the High Energy limit. The approximation results in sufficiently simple matrix elements, that these can be explicitly regulated, integrated and summed over any (relevant) multiplicity. This results in an explicit all-order resummation of the dominant contributions from wide-angle QCD radiation.

The building blocks of the HEJ framework ensure the correct leading logarithmic behaviour in the Multi-Regge Kinematic limit (aka. the High Energy Limit) of large invariant mass between all partons, for both the real and virtual corrections. The resummed $n$-jet rate is then further matched to tree-level accuracy for events with up to and including four jets, using a merging procedure for the soft radiation.

This procedure has so far been applied to the production of jets [64], $W$ plus jets [449], $Z$ plus jets and Higgs boson plus jets and has currently been implemented in a fully flexible Monte Carlo for the first two of these processes. The implementation integrates explicitly over any number of QCD emissions from a $(W, Z, H+)$ dijet system, and hence produces event samples for processes with two jets or more. Note that one has access to the momenta of all final state particles for every event and it is therefore extremely simple to restrict to a subset of the events if required, e.g. 3-jet exclusive events.

The HEJ resummation includes emissions at large transverse momentum which are increasingly important as the centre-of-mass energy of particle collisions increases. HEJ is currently the only available flexible Monte Carlo generator to obtain leading logarithmic accuracy in the limit of large invariant mass between emissions. However, the HEJ framework does not include any systematic resummation in the collinear limit. This is included in a parton shower, but a careful merging procedure is required to link one with HEJ, as there is significant overlap between the soft emissions included in each approach; the first steps in this direction have been taken for jet production [431] and are ongoing. In the current study though, only parton level predictions are given.

Estimate of Uncertainty The HEJ framework does not contain any tunable parameters other than the choice of renormalisation and factorisation scale (just like any fixed order calculation). In this study, in common with other approaches, we choose both of these to be given by the geometric mean of the transverse momentum of the jets:

$$
\begin{equation*}
\mu_{R}=\mu_{F}=\left(\prod_{j=1}^{n} p_{T}^{j}\right)^{1 / n} \tag{18.2.1}
\end{equation*}
$$

where the jets are defined according to the relevant cuts in each analysis. This is however only an arbitrary choice, as the framework admits any choice for the scale, including $H_{T}, p_{T}$ of the hardest jet and a fixed scale. For a given scale, $\alpha_{s}$ is evaluated according to the relevant PDF.

In common with standard convention, we calculate the scale variation by changing this scale by a factor of two in both directions. In principle, one could also include the PDF uncertainty, but this is not done in this study (as the scale uncertainty dominates). As described above, HEJ contains matching to tree-level accuracy for up to four jets. However, unlike the merging procedure in a showered sample, the merging scale here is not a free parameter. There is only one rational choice for the merging scale: the minimum $p_{T}$ of a jet in the relevant analysis. However, in an inclusive sample with at least two jets, one could use as a further estimator of uncertainty the variation obtained when matching to three and four jet LO matrix elements. This procedure will be studied in detail in Ref. [449], but in the present study, we quote the uncertainty only from the scale variation.

### 18.24 MADGRAPH + PYTHIA

MADGRAPH [165, 446, 163, 191] is a general purpose leading order matrix element (ME) generator, with a broad variety of models available and easily extensible thanks to its modular structure. The event generation is performed by the MADEVENT component, a tool implementing the Single Diagram Enhanced algorithm for multi-channel phase space integration. When a user provided process is specified, MADGRAPH automatically generates the amplitudes for all the relevant subprocesses and produces the mappings for the integration over the phase space. This process-dependent information is then used by MADEVENT, where the process specific code generated allows the user to calculate cross sections and to produce unweighted events. Once the parton level events have been generated, a traditional parton shower (PS) Monte Carlo library can be run on top of the MADGRAPH output to describe additional QCD radiation, and possibly allow to produce hadron level generated events if a suitable hadronisation model is then applied.

In order to avoid double counting of QCD radiation from the matrix element and the parton shower, the MLM matching approach is used in its ktMLM implementation provided by the MADGRAPH team [191].

For the present study MADGRAPH-5.1.1 [191] has been used for the matrix element generation, while the parton shower and hadronisation has been provided by PyTHIA 6.4.2.4 [400]. The $W+n$ jet process has been simulated up to 4 additional partons. The PDF used in both calculations has been

CTEQ6L1, and in the matrix element calculation the strong coupling costant has been setup to be equal to the one from the PDF used. The factorisation scale and the hadronisation scale are set to the W transverse mass, $m_{\perp, W}$. The parton level clusterisation scale xqcut has been set to 10 GeV , while the ME - PS matching scale qcut has been set to the optimal value of 20 GeV , determined ensuring the smoothness of the differential jet rate.

The Pythia settings have been defined according the so called Tune Z2, an adjustment of Tune Z1 described in [450] for CTEQ6L1, where the $p_{\perp}$ cutoff for the multiple parton interactions is set to $\operatorname{PARP}(82)=1.832$ obtained on top of LHC data as far as the underlying event and multiple parton interactions are concerned, while the fragmentation parameters are those optimized on LEP data by the Professor [451] team.

Estimate of uncertainties To estimate the uncertainties due to the factorisation scale and the renormalisation scale, which are set to $m_{\perp, W}$, we varied them simultaneously by a factor two. In addition we have independently varied by a factor two the ME - PS matching scale.

While applying these modifications, the total cross-section is kept fixed to the value obtained with the default parameters, 27.77 nb . That is because we are only interested in shape variations of the distributions, rather than in the total cross-section of the process calculated by MADGRAPH, which is accurate only at the leading order.

### 18.25 PoWhEG BOX + PYTHIA8

The Powheg Box [13] is a computer framework to ease the Powheg [416] implementation of new processes. It only requires as input the individual components of the NLO calculation under consideration, i.e., the Born process, its virtual radiative corrections and the real emission contributions. Then it automatically combines them, canceling the emerging soft and collinear singularities in the Frixione-Kunszt-Signer (FKS) subtraction scheme, and produces the required events. The Powheg Box is also a library, where previously implemented processes are available in a common framework.

For the present study we make use of the $W+$ jet implementation presented in [440].
The produced events are passed to PYthia8 [348] through the Les Houches interface [452] and showered with the default transverse-momentum ordered shower, vetoing further emissions harder than the one already present in the input events. This is achieved by setting the starting scale of the shower as the transverse momentum of the hardest emission 38

When multiple partonic interactions (MPI) are turned on, these are allowed to be harder than the first Powheg emission. Indeed, since the $W+1$ jet process is not accounted for in MPI, there is no over-counting.

Eventually, the relevant distributions are evaluated by interfacing the MonteCarlo output to the RIVET [360] analysis, for the two given sets of ATLAS and CMS cuts.

Since we have simulated events starting from a hard process where a $W$ is produced in association with one jet, only observables built from events where at least 1 jet is present will be shown.

Generation of predictions and estimate of uncertainties Predictions presented here are based on a merged sample of $4 \mathrm{M} W^{+}+j$ and $4 \mathrm{M} W^{-}+j$ weighted events, produced with the default Powheg Box choice of parameters. In particular, we have required a minimum cut $p_{\mathrm{T}}=5 \mathrm{GeV}$ on the associated jet at the generation level and, in order to enhance the statistical sampling of the high- $p_{\mathrm{T}}$ tail, we have further suppressed the rapidly rising contribution at low jet $p_{\mathrm{T}}$ by the factor $p_{\mathrm{T}}^{2} /\left(p_{\mathrm{T}, \text { supp }}^{2}+p_{\mathrm{T}}^{2}\right)$, with $p_{\mathrm{T}, \text { supp }}^{2}=100 \mathrm{GeV}$. The inverse of this factor enters the event weight.

[^222]We have adopted the Powheg Box default values for EW parameters, namely

$$
\begin{equation*}
M_{W}=80.398 \mathrm{GeV}, \quad \Gamma_{\mathrm{W}}=2.141 \mathrm{GeV}, \quad\left(\mathrm{ff}_{\mathrm{em}}\right)^{-1}=128.89, \quad \sin ^{2}{ }^{`} \mathrm{~W}=0.222645 \tag{18.2.2}
\end{equation*}
$$

and we have assumed a CKM matrix with a mixing between the first two generations only

$$
\begin{equation*}
\left|V_{u d}\right|=\left|V_{c s}\right|=0.975, \quad\left|V_{u s}\right|=\left|V_{c d}\right|=0.222, \text { and }\left|V_{t b}\right|=1 . \tag{18.2.3}
\end{equation*}
$$

Finally, we have resctricted the integration region to the interval $0<M_{W}<2221 \mathrm{GeV}$.
For the computation of the Powheg $\bar{B}$ function, the renormalisation and factorisation scale was chosen equal to

$$
\begin{equation*}
\mu_{R}=\mu_{F}=p_{\perp, j} \tag{18.2.4}
\end{equation*}
$$

where $p_{\perp, j}$ corresponds to the transverse-momentum of the (single) parton recoiling against the $W$ boson in the so-called underlying Born kinematics [417]. We have also run the code using

$$
\begin{equation*}
\mu_{R}=\mu_{F}=1 / 2\left(\sqrt{M_{W}^{2}+p_{\perp, W}^{2}}+p_{\perp, j}\right) \tag{18.2.5}
\end{equation*}
$$

but no relevant differences were observed with respect to the aforementioned choice, being the two scales similar for the $W+1$ jet processes at hand.

The scales entering in the evaluation of parton distribution functions and of the strong coupling in the Powheg Sudakov form factor are chosen to be equal to the transverse momentum of the PowHEG hardest emission [417, 386].

Scale-uncertainty bands obtained by varying the factorisation and renormalisation scales entering the $\bar{B}$ function by a factor of two in either directions are used as an estimate of the theoretical error associated to higher order missing effects.

The uncertainty due to the PDF choice was estimated generating events using three different sets (CT10 [255], MSTW2008 [262], and NNPDF2.1 [312]). The value of the strong coupling constant at $M_{Z}$ is consistently read from the PDF table used. The further showering performed by PYTHIA8 is instead performed with default PDF and $\alpha_{s}$ definitions, the difference being beyond the claimed accuracy of the calculation. In this study, we have used PYthia8, version 8.153.

### 18.26 Pythias

Pythia8 [348] is the latest incarnation of event generators of the Pythia family. At the heart of the generator are parton showers that evolve high-scale processes to the scale of hadronisation, by generating splittings with DGLAP splitting kernels. The splitting scales are ordered in relative transverse momentum [348, 447], and the phase space is constructed in a dipole-like manner in order to capture soft gluon coherence effects [453]. A key point of the evolution of partonic states in PYTHIA8 is that all perturbative components are interleaved [348, 447, 454], i.e. multiple partonic interactions, space-like and time-like showers are all generated in one transverse-momentum ordered evolution sequence. This means that due to the competition for phase space, all steps in the event generation are correlated. For a detailed discussion how parameters of the interleaved shower evolution are tuned to collider data, see [455]. Pythia8 with additional matrix element corrections has so far not been tuned to data. Since in [441], only very small differences were seen for LEP between PYTHiA8 with and without matrix element merging, we expect only small re-tuning effects in the parameters of the Lund string model [456]. Similarly, since we keep the low-scale modelling of PYTHIA8 largely intact, only small changes in the underlying event tuning are expected. We however expect that some re-tuning will be needed for jet shape data.

It should be noted that Pythia8 includes a selection $2 \rightarrow 1$ and $2 \rightarrow 2$ processes, as well as a limited variety of $2 \rightarrow 3$ processes, but does not contain a general ME generator. New processes, particularly for higher jet multiplicities, have to be made available in form of Les Houches Event (LHE)
[452] files. By virtue of matrix element corrections, Pythia8 describes the first emission in $\mathrm{W}+$ jets with the full matrix element probability. When introducing matrix elements with one additional jet within matrix element merging, this allows to fully cancel the merging scale dependence for the first emission, while small merging scale dependencies enter when including further jets. Current versions of Pythia8 include a general implementation of the CKKW-L matrix element merging prescription [445]. Please consult [441] for a detailed discussion of the implementation in PYTHIA8.

Generation of the predictions To generate predictions with stand-alone Pythia8 (i.e. without inclusion of matrix elements for W production in association with two or more jets), the built-in $q \bar{q} \rightarrow \mathrm{~W}$ matrix element in Pythia8 was used to generate the initial configuration. This was then evolved with to the hadronisation scale and the ensemble of partons hadronised using the Lund string model. For this study, we use the publicly available PyTHIA 8.157, with CTEQ6L1 parton distribution functions, and the associated Tune 4C. Since [441] showed a large dependence of the quality of the matrix element merging on whether rapidity-ordered emissions are explicitly forbidden in space-like showers, results are presented with and without enforced rapidity ordering.

The inclusion of matrix elements for additional jets into PYTHIA8 is achieved with Cккw-L merging. All merging tasks are handled internally in PYthiA 8.157, allowing for a high degree of automation. This means that the user only needs to supply

- Matrix element configurations in form of LHE files.
- An identifier giving the hard process of interest.
- A value of the merging scale. Facilities to allow the user to implement a her/his own merging scale definition are available.
For this report, matrix element configurations with additional jets were generated with MADGRAPH/ MadEvent [163], and read into Pythia8 in form of Les Houches Events. Pythia8 then derives all possible parton shower histories for an event, probabilistically chooses a history, and uses the reconstructed states and splitting scales to perform a re-weighting with Sudakov factors and $\alpha_{s}$ values. This means each event will have a weight

$$
\begin{aligned}
w_{\mathrm{CKKWL}}= & \frac{x_{n}^{+} f_{n}^{+}\left(x_{n}^{+}, \rho_{n}\right)}{x_{n}^{+} f_{n}^{+}\left(x_{n}^{+}, \mu_{F}^{2}\right)} \frac{x_{n}^{-} f_{n}^{-}\left(x_{n}^{-}, \rho_{n}\right)}{x_{n}^{-} f_{n}^{-}\left(x_{n}^{-}, \mu_{F}^{2}\right)} \\
& \times \prod_{i=1}^{n}\left[\frac{\alpha_{s}\left(\rho_{i}\right)}{\alpha_{\mathrm{SME}}} \frac{x_{i-1}^{+} f_{i-1}^{+}\left(x_{i-1}^{+}, \rho_{i-1}\right)}{x_{i-1}^{+} f_{i-1}^{+}\left(x_{i-1}^{+}, \rho_{i}\right)} \frac{x_{i-1}^{-} f_{i-1}^{-}\left(x_{i-1}^{-}, \rho_{i-1}\right)}{x_{i-1}^{-} f_{i-1}^{-}\left(x_{i-1}^{-}, \rho_{i}\right)} \Pi_{S_{+i-1}}\left(\rho_{i-1}, \rho_{i}\right)\right] \Pi_{S_{n}}\left(\rho_{n}, t_{\mathrm{MS}}\right)
\end{aligned}
$$

where $\rho_{i}$ and $x_{i}^{ \pm}$are the the reconstructed shower splitting scales and momentum fractions of the incoming partons in $\pm$ z-direction, and $\Pi_{S_{+i}}\left(\rho_{i}, \rho_{i+1}\right)$ the parton shower no-emission probability when evolving the state $S_{+i}$ from scale $\rho_{i}$ to $\rho_{i+1} . \alpha_{\text {sME }}$ gives the strong coupling used in the matrix element calculation. All reweighting factors are generated dynamically with help of the shower. The interleaved evolution of PYTHIA8 is accommodated by consistently including effects of multiple interactions into the no-emission probabilities. A detailed description of the formalism is given in [441].

As input for the current analysis, we have produced LHE files for $\mathrm{W}^{+}+$jets with up to four (three) additional jets at Tevatron (LHC) energies. The renormalisation scale in MADGRaPH was fixed to $\mu_{R}=\mathrm{M}_{\mathrm{Z}}$. For hadronic cross sections, CTEQ6L1 parton distributions (as implemented in LHAPDF [457]) have been chosen at a factorisation scale $\mu_{F}=\mathrm{M}_{\mathrm{W}}$, and the strong coupling in the ME was correspondingly fixed to $\alpha_{s}\left(\mathrm{M}_{\mathrm{Z}}\right)=0.129783$. To regularise QCD divergences and act as a merging scale, a cut in

$$
k_{\perp}^{2}=\min \left\{\min \left(p_{T, i}^{2}, p_{T, j}^{2}\right), \min \left(p_{T, i}^{2}, p_{T, j}^{2}\right) \frac{\left(\Delta \eta_{i j}\right)^{2}+\left(\Delta \phi_{i j}\right)^{2}}{D^{2}}\right\} \quad \text { with } \quad D=0.4
$$

and a cut value of $k_{\perp, \min }=t_{\mathrm{MS}}=15 \mathrm{GeV}$ has been applied to the matrix element.

Merged Pythia8 predictions are given for the default settings, i.e. using the parameters of Tune 4C, for Tune A2 [458], and for Tune 4C without enforced rapidity ordering (dubbed Tune X). Again, it should be noted that so far, no tuning including additional jets has so far been conducted.

Estimate of uncertainties To estimate uncertainties of a merged prediction of W+jets, it is interesting to study the dependence on the merging scale value. For this, we have generated LHE files with three different $k_{\perp, \text { min }}=t_{\text {MS }}$ cuts $\left(t_{\text {MS }}=15,30,45\right) \mathrm{GeV}$, and performed CKKW-L merging on these samples. Furthermore, to show the effect of tuning, the $t_{\mathrm{MS}}=15-\mathrm{GeV}$-sample was processed for two adequate tunes, Tune 4C and A2.

Uncertainties related to shower ordering In [441], it was shown that restricting shower emissions in Pythia8 to regions of phase space ordered both in transverse momentum and rapidity leads to nonnegligible effects in merged predictions. This can be seen as an effect of limiting the shower accuracy by reducing the phase space over which splitting kernels are integrated, meaning the accuracy of Sudakov form factors is impaired. Loosely speaking, if above the merging scale, the matrix element, integrated over the full phase space ${ }^{39}$, differs substantially from the splitting probabilities integrated over the allowed parton shower phase space, merged results will exhibit substantial merging scale dependencies. Such problems are obviously introduced if the parton shower phase space is heavily constrained.

Changing the phase space regions in which the shower is allowed to radiate thus allows us to estimate the uncertainties of the merging procedure in conjunction with the underlying shower. Particularly, this procedure can test the quality of the matrix element merging beyond the first few emissions, and give hints on how the shower resummation may be improved.

To emphasise the impact of the shower transition probabilities, we choose a fairly small merging scale ( $t_{\mathrm{Ms}}=15 \mathrm{GeV}$ ) to regularise the tree-level matrix elements for this investigation. Then, for each matrix element state, we generate all possible parton shower histories for a matrix element state, by clustering emissions. This is achieved by inverting the shower momentum- and flavour-mappings.

When merging matrix elements with rapidity-ordered showers, we investigate two ways of biasing the selection of a particular history, from which to generate the necessary Sudakov form factors:

1. In a "y-blind" sample, we do not include an additional discriminant based on rapidity. This means that - just like in the standard case - $\rho$-ordered will be preferred over $\rho$-unordered ones.
2. In a " $y$-conscious" sample, we pick histories with rapidity-unordered splittings only if no rapidityordered histories were found. Adopting this strict ordering criterion, histories ordered in $\rho$ and rapidity will be chosen predominantly, and only if no such history exists, histories un-ordered in either $\rho$ and/or rapidity are picked.
It should be noted that to the accuracy of the parton shower, both these prescriptions are equivalent, and switching the choice of histories gives a real estimate of the quality of the merging in conjunction the underlying shower. We believe that including this uncertainty gives a pessimistic view on how wide the range of predictions of one merged calculation can be, indicating that although standard by now, matrix element merging in Pythia8 should be applied with care. However, with reasonable settings, including additional jets can improve the description of multiple hard jets substantially.

### 18.27 SHERPA

ShERPA [425, 146] is a full-fledged event generator capable of simulating all aspects of particle collisions as they occur at particle accelerators such as the Tevatron or the LHC. It includes two independent matrix element generators, AmEGIC++ [147] and Comix [459], to generate cross sections and distributions

[^223]for final state multiplicities of up to six to ten particles. In the former one, methods to automatically generate dipole subtraction terms in the widely used Catani-Seymour scheme [236, 150] have been incorporated [448]; the SHERPA package also supports the BLHA [145] for the interface to one-loop programs such as BlackHat or GoSam. For parton showering, SHERPA employs an algorithm based on Catani-Seymour subtraction kernels, proposed in [460] and implemented in the SHERPA framework in [461]. For the hadronisation, SHERPA uses either its native hadronisation scheme, based on the cluster fragmentation model [462] and its implementation described in [463] or an interface to PYtHIA [400] providing access to the routines of the Lund string model [456]. Both have been successfully tuned to LEP data within the SHERPA framework, with a similar quality in describing the data. The hadron decays are also fully provided in the SHERPA framework, as well as QED final state radiation to both the $W$-boson and the hadron decays, simulated using the YFS approach [464, 465].

In this work, the most recent, publically available SHERPA version, SHERPA-1.3.1, has been used in two ways of running the simulation, namely

1. in the MEPs mode:

In this method, towers of LO matrix elements with increasing jet multiplicity, in the case at hand $W, W+1, W+2, \ldots, W+n_{J}$ jets, are merged in the spirit of [429, 430] to yield an inclusive sample. In fact, codes relying on such algorithms have been compared in a previous publication [439], which helped to establish and validate the methods and their various implementations. In contrast to the original implementation in SHERPA [466], which used analytical forms of Sudakov form factors etc., the current version of the method [426] directly uses the parton shower for Sudakov rejections etc. and is thus closer in spirit to the variant presented in [445, 467] for multijet merging.
2. in the MENLOPs mode:

This method can be understood as the combination of a matching of the parton shower to a NLO matrix element and a merging of additional towers of LO matrix elements with even higher jet multiplicities. Thus, in the case at hand, inclusive $W$ production calculated at NLO accuracy is merged, as above, with LO matrix elements for $W+1, W+2, \ldots, W+n_{J}$ jets. This method has been pioneered in [442, 443] where the implementation employed within Sherpa has been detailed in the second reference.

The respective settings and relevant details for both simulation modes are described below.

Sherpa in MePs mode In the MEPS mode Sherpa was run with up to $n_{J}=6$ jets in the matrix element evaluation including all possible massless (anti-)quark and gluon initial and final states. All matrix elements were generated using Comix. The MEPS-separation parameter was set to $Q_{\text {cut }}=20 \mathrm{GeV}$, for its precise definition see [426]. The scales are chosen as

$$
\begin{equation*}
\alpha_{s}^{k+n}\left(\mu_{\mathrm{eff}}\right)=\alpha_{s}^{k}(\mu) \cdot \alpha_{s}\left(p_{\perp, 1}\right) \cdot \ldots \cdot \alpha_{s}\left(p_{\perp, n}\right), \tag{18.2.6}
\end{equation*}
$$

wherein the relative transverse momenta $p_{\perp, i}$ are the nodal values of the final state partons of the $W+n$ parton matrix element as obtained from recombining it using the inverted splitting probablities given by the parton shower. The core scale $\mu$ is then chosen as the partonic centre-of-mass energy of the reconstructed core process, i.e. $\mu^{2}=\hat{s}_{2 \rightarrow 2}$ where $k=0$ in the process at hand. In all stricly perturbative setups a parton shower cutoff of $t_{0}=(0.7 \mathrm{GeV})^{2}$ has been used.

The parton shower cutoff and all fragmentation parameters of both the internal cluster hadronisation and the interfaced Lund string fragmentation models have been tuned to LEP data and give a similarly good description. Similarly, the parameters of SHERPA's MPI model have been tuned to Tevatron and LHC data using the CT10 [255] parton density parametrisation. These parameters are given in App. 18.71

Sherpa in Menlops mode In the MeNloPs mode Sherpa is run with essentially the same parameters as in the MEPs mode, described in the previous subsection. Hence, $n_{J}=6$ and $Q_{\text {cut }}=20 \mathrm{GeV}$. To be able to describe the inclusive $W$ production process at NLO accuracy, AmEGIC++ was used for all parts of the NLO $W$ production matrix elements (supplemented with a hardcoded one-loop matrix element from the internal library) and the LO $W+1$ parton matrix element. Consecutively, the scales were chosen as above with $k=0$ for all tree-level parts and $k=1$ for the real and virtual corrections entering the next-to-leading order correction of the core process. All non-perturbative parameters remain unchanged wrt. the MEPS mode.

Estimate of uncertainties In order to estimate the uncertainites of the SHERPA predictions, the following procedures have been applied:
(A) PDF uncertainties:

Unlike in the PDF4LHC presciption [468], here only the central predictions of the three NLO PDFs, CT10 [255], MSTW2008 [262] and NNPDF2.1 [312] are compared to estimate the PDF uncertainties. The different parametrisations of PDFs as well as their corresponding value of $\alpha_{s}$, both its value at $M_{Z}$ and its running, enter in the calculation of the matrix elements, the parton shower and the underlying event.
(B) Scale uncertainties:

In a global manner, all scales, renormalisation and factorisation scales are simultaneously modified by the canonical multiplication with 2 and $1 / 2$. This, however, is not only applied to the evaluation of the matrix elements but also to that of the parton shower, the hadronisation, the underlying event simulation and the hadron decays. Regarding the matrix-element evaluation, the MEPs default scale choice forms the starting point for the scale variations to be executed.
(C) Hadronisation uncertainty:

Here the intrinsic modeling uncertainties are evaluated by changing the hadronisation model operating on SHERPA's parton shower final states, namely switching from SHERPA's default cluster hadronisation to PYTHIA's string fragmentation. For both schemes, an independently tuned set of parameters has been employed to perform the parton-to-hadron transition.
(D) Underlying event uncertainty:

To this end the tune of the underlying event based on using the CT10 PDF has been modified such that the plateau of the number of charged particles and sum of transverse momenta in the transverse region are increased or decreased by $10 \%$. This change in the amount of MPI activity is accomplished by varying the $\sigma_{\mathrm{ND}}$ correction factor (SIGMA_ND_FACTOR) by -0.04 or +0.05 , respectively.

### 18.3 Results

In this section we compile results for the individual codes for a number of representative observables at the different levels of the simulation. It should be noted, though, that in all results presented in this section PDF uncertainties have been estimated by typically varying only over a few different sets rather than employing the full procedure as suggested by the PDF4LHC accord [468].

### 18.31 BLACKHAT + SHERPA

The following results have been obtained with BlackHat+SherPa. Uncertainties due to the factorisation/renormalisation scale variation and the that due to the PDF uncertainties are shown. The yellow band corresponds to the addition in quardature of these two uncertainties and the statistical estimation on the integration error. All observables are defined using the ATLAS cuts, cf. App. 18.6.

Fig. 64 displays the inclusive cross section for a $W$ boson in association with $n$ jets, where $n=1,2,3,4$. A NLO computation of $W+4$ jets also provides a leading order calculation of the $W+5$
jets rate, but since it is not at NLO accuracy we refrain here from including it.
In all the plots presented in this section the uncertainties are dominated by the uncertainty arising from the scale variation (it is not the case when the central scale of the process is chosen close to a local maximum, in which case the upper boundary of the scale variation is very close or identical with the central value, as can be seen from the plots corresponding to $W+3,4$ jets). This is partially due to the fact that for the assessment of the PDF uncertainty only error sets have been employed that are closely related to the central set. In addition, the functional form of the scale definition as given by the kineamtics of the final state has not been changed, but rather the emerging scales $\mu_{F}$ and $\mu_{R}$ have been multiplied in parallel by factors of 2 and $1 / 2$.


Fig. 61: Pseudo-rapidity and transverse momentum distributions for the first jet in inclusive $W+1$ jet production (upper panel), for the second jet in inclusive $W+2$ jet production (central panel), anf for the third jet in inclusive $W+3$ jet production (lower panel).


Fig. 62: Pseudo-rapidity and transverse momentum distributions for the fourth jet in $W+4$ jet production.


Fig. 63: HT distributions for event with at least one (top left), two (top right), three (bottom left) or four (bottom right) jets.


Fig. 64: Inclusive cross section for $W+n$ jet production.

### 18.32 GoSAM + SHERPA

The setup described in the previous section for the analysis using GoSAM+SHERPA gives the following theoretical uncertainties. The plots show that in general the scale uncertainties are bigger then the PDF uncertainties and that the renormalisation scale dependence is usually bigger then the dependence on the factorisation scale. To illustrate the decrease in the scale uncertainty given by the NLO calculation we also include the distributions for the pseudo-rapidity and transverse momentum of the second hardest jet, which have only tree-level accuracy. All observables shown are defined using the ATLAS cuts, cf. App. 18.6 Note that errors in the 2 -jet configuration are increased w.r.t. those provided by BLACKHAT+SHERPA, since here only $W+1$ jet configurations are dealt with at NLO, and the 2 -jet configurations therefore are descibed at LO only.


Fig. 65: Pseudo-rapidity and transverse momentum distributions for the hardest jet.


Fig. 66: Pseudo-rapidity and transverse momentum distributions for the second hardest jet. This distribution have formally leading order accuracy and have therefore a much larger scale dependence than the same distribution for the hardest jet, for which a genuine NLO prediction is available.


Fig. 67: HT distributions (left) and $\Delta R$ between lepton and hardest jet (right) for events with at least one jet.

### 18.33 HEJ

This section contains the predictions from the High Energy Jets (HEJ) event generator. This gives predictions for the production of a $W$ boson in association with at least two jets. Throughout, we show results for CTEQ, MSTW and NNPDF parton distributions. We show a scale uncertainty band only for the first of these for clarity. The results for the other two are very similar. The yellow band in the ratio panel shows the statistical uncertainty in each case. The scale variation is seen to be dominant over the statistical uncertainty and the differences in choice of pdf. All observables are defined using the CMS cut definitions, cf. App. 18.6

As discussed in Sec. 18.23, the resummation contained in the HeJ framework is supplemented with a merging procedure to ensure tree-level accuracy for events with up to and including four jets. This leads to the larger drop from the four jet to the five jet cross section, compared to the drop either from


Fig. 68: The Hes prediction for the distribution of the transverse mass of the $W$ boson (top left) and for the angle between the hardest jet and the charged lepton from the decay of the $W$ boson (top right), the transverse momentum of the hardest jet (bottom left) and for the $H_{T}$ distribution (bottom right) in events where a $W$ boson was produced in association with at least two jets.


Fig. 69: The Hes prediction for the cross sections of $W$ plus $n$ jets.
three-jet to four-jet, or from five-jet to six-jet. This can be clearly seen in Fig. 69

### 18.34 MadGraph + PYthia

The following results have been obtained with MadGraph+Pythia. Uncertainties due to the factorisation and renormalisation scale and MEPs matching scale are shown for results on hadron level including UE and QED final state radiation. A comparison of results on parton shower level, hadron level, hadron level including UE, and hadron level including UE and QED final state radiation, is also presented. All observables shown are defined using the CMS cuts, cf. App. 18.6.

From these results we can conclude that the largest uncertainty on all observables is due to the factorisation and renormalisation scale. In addition to that, a large effect is found by switching off the final state QED radiation, while only a small difference is oberved between results at the shower level and all other results prior to the QED radiation.


Fig. 70: MadGraph + Pythia results for $W$ transverse mass.


Fig. 71: MADGraph+PYTHIA results for $\Delta R$ between lepton and hardest jet.


Fig. 72: MadGraph+Pythia results for for $p_{\perp}$ of hardest jet (top), number of jets (middle) and $H_{T}$ of events with at least 2 jets (bottom).

### 18.35 Powheg Box + Pythia8

In this section we show results obtained by running the Powheg Box implementation of $W+1$ jet together with Pythia8. In all the following plots of this section, CMS analysis cuts have been enforced, see App. 18.6. For this study, in the left panels of Figs. 73.75, we show uncertainties obtained from variations of renormalisation and factorisation scales by a factor of two in either directions and by choosing different PDF sets in the computation of the hard scattering. Results are shown at the final level, after the shower, the hadronisation and the inclusion of MPI, all performed by PYTHIA8. In general, we notice that the uncertainty due to scale variations is greater than the changes in the results due to different PDF choices.

In the right panels of Figs. $73 / 75$ we show our results at different stages of the simulation, for a fixed PDF set (chosen to be CT10). The stages considered include from the first emission level up to the full showered events in PYTHIA8, including MPI and also effects due to QED radiation off leptons and quarks. Various stages of the simulation have been obtained setting the PYTHIA8 switches as reported in Sec. 18.73 .

We recall here that results should be considered to be physical only after the the hadron level is reached (possibly including MPI and QED effects). In particular, we stress that the results at the parton level are obtained considering only the POWHEG first emission, and they are therefore only intermediate: indeed at this stage only the hardest radiation has been generated and effects due to further showering are not yet taken into account.

For most of the observables results do not show large variations going from a simulation level to another. In particular, for truly NLO predictions such the plots in Fig. 74 or the bin $n_{\text {jet }}=1$ of Fig. 73 , the major effects that arise at each successive stage of the simulation are a change in the normalisation, due to a slightly different number of events passing the analysis cuts when multiple emissions are allowed, and a moderate shape distortion in the low end of the spectrum. Both these effects may be attributed to multiple QCD radiation due to Sudakov effects introduced by the parton shower. As expected, these effects are of the same size, or smaller, than the theoretical uncertainty due to scale and PDF's variations, when propagated to the hadronic level. Similar effects are also observed when the QED radiation is turned on. In this case, results are lowered as a consequence of the cuts on the lepton transverse momentum and rapidity.

Due to the requirement of having at least two jets, the remaining observables are predicted only at leading order or with leading log accuracy by the Powheg simulation of $W+1$ jet. This is also reflected


Fig. 73: The number of jets, as predicted by Powheg Box + Pythia 8 .


Fig. 74: The hardest jet transverse momentum distribution (upper plots), the $\Delta R$ separation (middle plots) and the invariant mass $m$ (lower plots) of the hardest jets and the hardest lepton, as predicted by Powheg Box + Pythia8.


Fig. 75: The transverse momentum $p_{\perp}$ of the next-to-hardest jet, the scalar sum of the jet transverse energy $H_{T}$ of events with at least 2 jets and the sum of the transverse energies of all the particles in events with 2 or more jets, as predicted by Powheg Box + Pythia8.


Fig. 76: Comparison between predictions using different PYTHIA8 tunes, at hadron level with MPI, as predicted by Powheg Box + Pythia8.
in the larger band associated with the scale variations.
Observables such as $H_{T}$, the scalar sum of the transverse energy of the jets for events with two or more jets, show an enhancement in the high- $H_{T}$ tail. This effect mostly arise as a consequence of the showering, since the successive stages do not change the predictions any longer. The same behaviour, even more enhanced, is also observed in the scalar sum of the transverse energy of all particles, always in events with two or more jets.

In Fig. 76 we instead compare the effect of using different PYTHiA8 tunes on our predictions, obtained in this case at the hadron level, including MPI. Essentially all the observables turned out to be extremely stable under the variations of the PYthia8 tune, as shown in Fig. 76. Major differences only appears for the beam thrust, when it is defined at the particle level (see App. 18.62).

### 18.36 Pythias

For this study, PYthia8 has been run stand-alone and including matrix elements with additional jets. Note that in PYthia8, multiple interactions are interleaved with space- and time-like showers, meaning that in general, MPI and parton showers cannot be disentangled by just switching off secondary scatterings. When referring to "Hadron Level", we mean after the interleaved evolution (including QED


Fig. 77: Tuning variations for Pythia8 at hadron level. The plots show the $H_{T}$-distribution when requiring at least two jets (upper left), the $p_{\perp}$ of the hardest jet (upper right), the $\Delta R$-separation of lepton and the hardest jet (lower left), and the number of jets (lower right). The lower insets show the ratio of the samples in the upper half to ME3PS (Tune 4C, y-blind treatment). All merged plots are produced with a merging scale of $t_{\mathrm{MS}}=15 \mathrm{GeV}$.
splittings), and after hadronisation. For the sake of comparison, "Shower Level" indicates results after (interleaved) final- and initial-state radiation, switching multiparton interactions off. All results presented in this section are generated with CTEQ6L1 parton distributions for protons colliding at $E_{\mathrm{CM}}=7000$ GeV . Cккw-L-merged samples include up to three additional jets, taken from MADGraph/MadEvent.

Fig. 77 exemplifies how changes in the tuning of the event generator can affect the outcome of merged calculations in PYTHIA8. For this, we produce predictions for Tune 4C [455] and Tune A2 [458]. In general we observe only modest shape changes of up to about $20 \%$ in observables, when comparing the two merged predictions, lending confidence to the statement that the tuning did not artificially produce hard scale physics. Normalisation changes between 4 C and A2 can be explained by a difference in Sudakov suppression: Since Tune 4C integrates the splitting kernels over a smaller region of phase space, the suppression generated by trial showers is less pronounced. The increase in the number of jets in Tune A2 with respect to Tune 4C, after the third jet, is expected, because the generation of the fourth jet is handled solely by the parton shower. Since 4C allows less phase space for these emissions by


Fig. 78: Variation of the merging scale value for Pythia8 at shower level. The plots show the $H_{T^{-}}$ distribution when requiring at least two jets (upper left), the $p_{\perp}$ of the hardest jet (upper right), the $\Delta R$-separation of lepton and the hardest jet (lower left), and the number of jets (lower right). The lower insets show the ratio of the samples in the upper half to ME3PS for $t_{\text {MS }}=30 \mathrm{GeV}$. All plots are generated using Tune 4C (y-blind treatment).
enforcing rapidity ordering, A2 will look harder. It is debatable whether including rapidity ordering into the tuning makes the tune mimic hard scale effects. The scales at which the fourth jet is produced are certainly close to the scale of (hard) multiple interactions, which is in turn closely connect to soft physics. Although the enforced rapidity ordering in Tune 4C might be considered questionable, we here take the pragmatic approach of considering the evolution both with and without enforced rapidity ordering. From the fact that up to three jets, the merged predictions of Tune 4C and Tune A2 only differ in normalisation, we anticipate that the effect of rapidity ordering will be reduced by merging more jets, since then, the number of jets above a cut-off will be dictated by the matrix element.

In Fig. 78, we investigate the impact of changes in the merging scale value. Again, we mainly see normalisation changes and only small changes in shape, which in most cases are smaller than changes due to different tunes. The $R$-separation between lepton and hardest jet $\Delta R$ (lepton, hardest jet) shows significant shape changes above $\pi$. This again is an effect of Tune 4C, and is greatly reduced in Tune A2 $2^{40}$, as

[^224]

Fig. 79: Variation of the criterion employed to favour "ordered histories" in Pythia8 at shower level. The plots show the $H_{T}$-distribution when requiring at least two jets (upper left), the $p_{\perp}$ of the hardest jet (upper right), the $\Delta R$-separation of lepton and the hardest jet (lower left), and the number of jets (lower right). The lower insets show the ratio of the samples in the upper half to ME3PS (Tune 4C, y-blind treatment). All merged plots are produced with a merging scale of $t_{\mathrm{MS}}=15 \mathrm{GeV}$.
can be inferred from the tune variation. However, even in Tune A2, small shape changes remain, with the change becoming less pronounced when comparing two large merging scales. We take this as an indication that the shower splitting probability - giving radiative contributions to $\Delta R$ (lepton, hardest jet) $>\pi$ for high $t_{\mathrm{Ms}}$ - and the the matrix element, which fills the same region in for the low merging scale case, are indeed different from the second jet on. This also explains the difference between Tune 4C and Tune A2, which differ by the phase space regions over which the splitting kernels are integrated.

Finally, in Fig.79, we address the interplay of matrix element merging and ordering in the underlying shower more carefully. The effect of different choices manifests itself again mainly in changes of the normalisation of the plots, and is comparable in magnitude to the impact of merging scale variations. At first, the changes may seem counter-intuitive, and need clarification. For this, it is important to remember the definition of " y -blind" and " y -conscious" in section 18.26 . The y -blind treatment will - irrespectively of rapidity configurations - mainly choose histories ordered in the shower evolution variable $\rho$, and only

[^225]pick $\rho$-unordered histories if no other ones have been constructed. However, in the y-conscious approach, once no history ordered both in rapidity and $\rho$ is found, one amongst all un-ordered histories is chosen probabilistically, irrespectively of the history being y-/ $\rho$-/or y- and $\rho$-unordered. Since the ordering criterion is stricter, un-ordered histories will be chosen more frequently, meaning that $\rho$-unordered ones will also contribute more, compared to the y-blind case. Matrix element states with no ordered histories will have a number of jets at very similar scales, so that the Sudakov suppression generated by trial showers will be smaller. Moreover, for matrix element states in which the last reconstructed splitting is unordered, the parton shower will be started at the larger of the unordered scales ${ }^{41}$, which can result in a slightly harder spectrum of resolved parton shower jets. Because $\rho$-unordered states are picked more often when requiring a tighter ordering criterion, this leads in visible differences. The y-conscious method might seem somewhat artificial, considering that it introduces a larger dependence on states outside the range of even the $y$-unordered shower variant. Nevertheless, the $y$-blind and $y$-conscious prescriptions are equivalent to the accuracy of the (y-ordered) shower, so that both should be investigated when assessing the quality of the merging. From the visible changes, we can infer that different treatments of formally sub-leading effects do matter. For the y-ordered evolution, these are more visible since the accuracy of the shower itself is worse, so that the effects of including matrix element states cancel to a lesser degree. It is interesting to note that the deviations between the different prescriptions are considerably smaller if the merging scale is increased, again hinting at a reduced shower accuracy if the evolution is ordered in multiple variables.

Fig. 79 further shows distributions labelled Tune $X$, which have been generated by using Tune 4 C , removing the rapidity constraint on space-like emissions, and treating histories y-blind. Results of these runs, as expected, closely follow Tune A2. The outcome of both Tune A2 and Tune X differs only slightly from the Tune 4 C (y-blind) curves, consolidating the conclusion that shifting fractions of $\rho$-un-ordered histories are responsible for the deviations between the y-blind and y-conscious methods. As in the discussion of tuning variation, the similarity in the results of the merged calculation for Tune 4C and Tune A2 breaks down once we examine jets that are solely produced by the shower, i.e. starting from the fourth jet.

### 18.37 SHERPA

As described in Sec. 18.27 , SHERPA has been run in two modes for this comparison of LHC predictions. The results for the conventional merging of towers of tree-level matrix elements, SHERPA MEPS, are presented in Sec. 18.37 while the results of its enhancement to NLO accuracy in the core $W$ production process, Sherpa MeNloPs, are displayed in Sec. 18.37 . As detailed earlier, all parameters have been chosen identically otherwise. The precise requirements regarding the event selection and the definitions of the observables used in this comparsion follow the CMS cut specifications and can be found in App. 18.6.

SHERPA MEPS Figs. 80,83 show the results as obtained by running SHERPA in the MEPS mode for a variety of inclusive and multi-jet observables at different levels of the event generation. All central results are displayed together with their respective uncertainties related to the different sources listed in Sec. 18.27. The layout in all figures is the same: the upper left and right panels respectively show the matrix element level and parton shower level predictions for a given observable. The matrix element level is defined as the event generation phase right before the parton showering. For the MEPs approach this means that modifications necessary for the procedure to work like $\alpha_{s}$ reweighting and Sudakov rejection have been already included at this level. The predictions presented in all centre panels were generated after enhancing the event generation to include corrections induced by the parton-to-hadron transition and decays of the therein produced primordial hadrons. On top of these soft physics effects, one has to also

[^226]

Fig. 80: SHERPA MEPS. Uncertainty of the transverse mass of the reconstructed $W$ on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 81: Sherpa MePs. Uncertainty of the angular separation of the charged lepton and the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 82: SHERPA MEPS. Uncertainty of the transverse momentum of the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 83: Sherpa MEPs. Uncertainty of the inclusive jet multiplicity on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.
account for multiple parton interactions. The results in the centre right panels of all figures incorporate these additional corrections. Finally, all plots to the lower left show the most complete hadron level predictions, which were obtained by adding to the event generation QED radiation effects as occurring in the decays of the vector boson and the hadrons. To allow a direct comparison of the impact of the consecutive event stages, the way the central results change is summarized in all plots to the lower right of Figs. 80.83 . In these, as in all other panels, the main plots are supplemented by ratio plots stressing the magnitude of the differences and uncertainties. Note that the yellow band throughout illustrates the statistical uncertainty on the central event sample.

Apart from the summary plots at the lower right, all other cases depict predictions documenting the uncertainty of the central predictions at the different levels of event generation. These uncertainty estimates are gained following the procedures outlined in Sec. 18.27. At all event simulation phases, the scales are varied as described under this section's point (B). Note that the variation is applied to all phases used to make up the respective central (or default) sample, which is taken as the reference under all circumstances. For the matrix element level, parton shower level and full hadron level results, PDF variations according to point (A) are shown in addition, whereas for the centre panel plots, the focus is on the outcomes of the model and tune variations instead, as specified in point (C) and point (D) of Sec. 18.27. Notice that the lower left panels also contain the outcomes of scale variations utilizing the alternative PDFs mentioned under point (A); they are much alike the ones stemming from the default set.

As an example for an inclusive observable the transverse mass of the reconstructed $W$ boson is shown in Fig. 80. The scale uncertainties amount to $\sim 15 \%$ at all generation levels, whereas the uncertainties due to the choice of PDF are much smaller. Similarly, the hadronisation uncertainty is negligible. The $m_{\perp, W}$ observable however is more sensitive to the tuning of the MPI model as can be seen from the $\pm 10 \%$ envelope in the centre right plot of Fig. 80. The uncertainty is of the same order as for the scale variations, which generally are more pronounced in the soft region. When considering the impact of each perturbative and non-perturbative event stage (see the plot to the lower right), it is the MPI corrections that are largest in the region of $m_{\perp, W}<m_{W}$, ranging up to $\sim 30 \%$ wrt. the matrix element level prediction. They are small above $m_{W}$. In this region the dominant effect comes from the QED corrections, which themselves are rather small, but they lead to a contamination of the electron isolation. The application of the isolation cuts then yields a reduction of the overall normalisation of the event sample. Finally there is a small shift towards lower transverse masses, pronouncing the deviation in the tail of the distribution somewhat further.

Fig. 81 and Fig. 82 depict observables that require the presence of at least one jet. In the former the geometric separation, $\Delta R$, between the hardest jet and the electron is shown, while in the latter, focus is on the transverse momentum, $p_{\perp}$ of the hardest jet only. As before the dependence of the predictions on PDF and hadronisation model changes remains negligible. While the scale dependence of the $\Delta R$ and $p_{\perp}$ variables increases to $\sim 30 \%$, the uncertainty due to the tuning of the MPI model decreases to $\sim 5 \%$ when compared to the findings concerning the more inclusive observable considered above. In both cases the reason for the sensitivity change obviously lies in demanding at least one (hard) jet. The scale uncertainties primarily result from changes in the overall cross section. Again, comparing the results of the different event stages, one clearly observes the large impact parton showering has on modifying the matrix element level predictions. The non-perturbative effects go in the same direction amplifying the parton shower effects, but as expected this amplification turns out to be rather mild in the well separated and/or hard phase space regions. QED corrections only play a minor role, and are far less important than for the $m_{\perp, W}$ variable.

In Fig. 83 one of the simplest examples of a multi-jet observable is presented, namely the distribution of the inclusive $W+n$ jet cross sections as a function of $n_{\text {jet }}$. Qualitatively, the parameter and model dependencies of the predictions are found to behave as for the inclusive one-jet variables. As one would expect, the scale uncertainties subsequently increase with the order of the jet bin. The same can be noticed for the variation of the PDFs used in the calculation - even though here the effect is considerably
smaller.

Sherpa MeNloPs Following the outline of the previous subsection, Figs. 84.87 compile the results, which were obtained by executing SherPa in the MENLoPs mode, cf. Sec. 18.27. The presentation is based on the same set of figures where the selection of the observables has been taken as in the MEPS case. Again, all (central) predictions are examined towards their scale, PDF, non-perturbative modeling and QED simulation dependence. One small difference has to be pointed out: the plots to the lower left now depict exclusively to what extent the additional QED corrections modify the outcomes including multiple parton interactions and hadronisation effects.

Fig. 84 shows the transverse mass of the reconstructed $W$ boson. In the MENLOPs approach, this observable is described at NLO accuracy, which leads to a reduction of the associated scale uncertainties. The scale variation results for $m_{\perp, W}$ nicely confirm this expectation as can be seen in the upper four plots of Fig. 84. The deviations from the central prediction are much smaller than those found for the MEPs scenario exhibited in Fig. 80, they now are of similar magnitude as the PDF uncertainties. While the scale dependence is reduced, PDF and MPI tune variations as well as QED corrections manifest themselves as in the MEPS case. In particular, the discussion around Fig. 80 explaining the effects of extra QED emissions (as being most relevant in the $W$ decay) can be used to understand the findings illustrated in the bottom left panel of Fig. 84

The MENLOPs method primarily improves the precision of the description of the core process, here the description of the $W$ production process. One also benefits from improving the overall normalisation. However, processes with additional partons in the final state are described in the MENLoPs approach at the same level of accuracy as in the MEPS approach - in both cases by tree-level matrix elements. Thus, the one-jet observables, $\Delta R$ between the lepton and leading jet and the $p_{\perp}$ of the leading jet, and their related uncertainties turn out to be predicted in a very similar manner. This can be clearly observed by comparing Figs. 85486 with Figs. $81 / 82$. Unlike the findings for $m_{\perp, W}$, it particularly can be noticed that the scale dependence associated with the one-jet observables shown here remains unchanged when compared to the respective MEPS results.

Fig. 87 depicts the distribution of the inclusive $W+n$ jet cross sections as obtained for the MeNloPs case. Using the above reasoning, one can understand these results as for the one-jet variables. Note that the scale dependence of the zeroth jet bin shows the expected decrease owing to the NLO accuracy underlying the description of the core process.

Fig. 88 finally, highlights the evolution and uncertainties of two definition of the beamthrust, cf. App. 18.6 a physical observable summing over all final state particles excluding the $W$-constituent lepton and a pseudo-observable including the $W$ itself. For both observables small perturbative uncertainties are completely burried underneath much larger non-perturbative effects and modelling uncertainties, an effect also seen in results from the Powheg Box+Pythia simulation, cf. Fig. 76. This can only be interpreted as this observable being dominated by non-perturbative effects and in particular the underlying event, which somewhat invalidates statements about the merit of this observable in a clean determination of initial state radiation effects made in [469, 26].


Fig. 84: Sherpa MeNloPs. Uncertainty of the transverse mass of the reconstructed $W$ on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 85: Sherpa MeNloPs. Uncertainty of the angular separation of the charged lepton and the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 86: Sherpa MeNloPs. Uncertainty of the transverse momentum of the hardest jet on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 87: Sherpa MENLoPs. Uncertainty of the inclusive jet multiplicity on the matrix element level (upper left), after parton showering (upper right), including hadronisation correction (centre left), multiple parton interactions (centre right), and QED corrections (lower left). The lower right panel shows the evolution of the central value.


Fig. 88: Sherpa MeNloPs. Evolution and uncertainty of two definitions of the beamthrust, calculated using all particles not constituting the $W$ (left) and including the $W$ (right). Exemplary, the combined PDF and scale uncertainty on the matrix element level prediction (yellow) and the modeling uncertainty of the hadron level prediction (blue) are shown.

### 18.4 Comparisons

In this section we compare the results of different tools with each other. While the aim of this study was to have a fairly tuned comparison with as many aspects of the calculations as possible being centrally defined, there are still important residual differences in the various results. Obviously, the different codes produced results at different stages of the simulation, which are not always directly comparable; in addition, some of these stages are not very straightforward to obtain: for instance, running PyTHIA8 without multiple parton interactions included in the interleaved showering obviously changes the overall logic of the parton shower model of this code. In addition, other, more obvious differences occur, ranging from inconsistent choices of PDFs to different strategies in scale setting procedures. For the case of the PDFs, by directly comparing results obtained with BlackHat+SHERPA using CTEQ6.6 and with GoSAM+SHERPA using CT10, it appears as if at NLO these differences are minor. However, it is not clear how much of the differences between MADGraph+PYTHIA and PYTHIA8, which both employ CTEQ6L1, and the other codes, which employ NLO PDFs, can be attributed to differences in PDFs.

In addition, results obtained with the NLO codes typically include at least one jet - Powheg Box+Pythia8 and GoSam+Sherpa take $W+1$ jet at NLO as their core process - while Hej starts at $W+2$ jets, and BlackHat+Sherpa presents results for up to 4 jets accompanying the $W$ boson in different jet bins. Obviously, on the other hand, the multijet merged samples of MadGraph + PYthia, Pythia8 MePs and Sherpa include LO matrix elements for up to 3 to 6 jets.

In the plots in this section each code is shown with a yellow error band, which is the envelope of the variations presented in Sec. 18.3. The only exception is BLACKHAT+SHERPA, which is shown with a blue error band. In the ratio plots the codes are plotted relative to BLACKHAT+SHERPA, also at the parton shower level.

### 18.41 Inclusive observables

In this section we present some inclusive observables, which are typically all obtained from codes employing multijet merging. By and large, all codes agree in the shapes of the $m_{\perp, W}$ distribution at different stages, although there are sizable differences in the respective normalisation of the samples.


Fig. 89: Transverse mass of the reconstructed $W$ on all levels of the simulation, for the exact definition see App. 18.62 and for the cuts employed in the analysis App. 18.61 Note that PyTHIA8 and MadGraph+PyTHia use the CTEQ6L1 pdf, while Sherpa uses CT10.

### 18.42 Observables with at least one jet

As a first and fairly telling observable the $p_{\perp}$-spectrum of the hardest jet is compared, cf. Fig. 90, At the parton level, the results of the NLO calculations - BLACKHAT+SHERPA and GOSAM+SHERPA- agree nearly perfectly with each other and within about $20 \%$ with the multijet merged samples of SHERPA, both at LO (Sherpa MePs) and in the MeNloPs (Sherpa MenloPs) sample. The increase of the latter with respect to the former at relatively low transverse momenta of about 50 GeV or below can probably be related to the different scale definition in the argument of the strong coupling, where the NLO calculations choose $\mu_{R}^{2}=\left(H_{T}^{\prime} / 2\right)^{2} \approx M_{W}^{2} / 4+p_{\perp, j}^{2}$ while in the SHERPA simulation the transverse momentum of the jet has been chosen. Clearly, for small transverse momenta this will lead to visible differences. Going from the matrix element to the parton shower level typically leads to the jets becoming softer and to losing some of them, due to partons emitted outside the jet and a corresponding energy loss. This explains why the SHERPA distribution at the shower level is softer than the NLO result, and thus the SHERPA result at the matrix element level, although the size of the difference seems to be larger than one would naïvely expect. This finding is, however, somewhat at odds with the results obtained from MADGRAPH+PYTHIA, which seem to be slightly harder in shape and significantly larger in normalisation. The PYthia8 MEPS sample, on the other hand, has a smaller one-jet inclusive cross section than SHERPA, but the jet spectrum exhibits a somewhat harder tail, corresponding to a shape difference of about 30$40 \%$ with respect to both the Sherpa results. The same finding, a somewhat harder tail, is also true for the Powheg Box+Pythia8 results. The same trends can be also found at the hadron and hadron + MPI level. For the Powheg Box result the difference can be attributed to the usage of a scale defined at the "underlying-Born" level (cf. Sec. 18.25 for more details). Indeed it has been checked explicitly that a NLO computation performed with the same scale choice used in Powheg Box gives a result in complete agreement with the POWHEG Box result shown here. Clearly, the differences between different


Fig. 90: Transverse momentum of hardest jet on all levels of the simulation, where jets are reconstructed using the anti- $k_{\perp}$ with $R=0.4$ within $|\eta|<4.4$ (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BlackHat+ShERPA (on matrix element level).
calculations and codes exhibited here deserve a more in-depth study, which, unfortunately, is beyond the scope of this comparison.

Similar findings are also true for the next observable, the $\Delta R$ distribution between the lepton stemming from the $W$ decay and the hardest jet displayed in Fig. 91. Again, the two Sherpa samples are compared with the two NLO samples, this time exhibiting a sizable shape difference towards an increase at smaller and a decrease at larger distances of about $40 \%$ relative cross section. While higher jet configurations typically tend to be a bit more central, it seems far-fetched to attribute this difference only to them. At the same time, large differences in $R$ are most likely due to jets which are pretty much forward ${ }^{42}$. This region of phase space for jet production, however, is known to be quite susceptible to mismatches in scale and/or PDF definitions. However, it is worth noting that this difference vanishes almost completely at the parton shower level. The Pythia8 MEPs sample, despite a sizable difference in cross section, appears to follow the shape of the NLO and SHERPA results. Further comparing these results to those of the other codes at the shower level suggests that the MadGraph+Pythia merged sample, apart from a drastically enhanced cross section, also shows an enhancement in shape at smaller $\Delta R \leq 2$ w.r.t. the NLO result. Interestingly enough, the Powheg Box+Pythia8 sample exhibits the

[^227]

Fig. 91: $\Delta R$ between hardest lepton and hardest jet on all levels of the simulation (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).
opposite behaviour: while the cross section seems fairly consistent with the SHERPA and the NLO ones, the shape shows some enhancement of up to $40 \%$ at large distance $\Delta R$, which following the reasoning for the jet $-p_{\perp}$ spectrum may also hint at being due to a difference in the definition of scales. As before, the same trends visible at the parton shower level can also be found at the hadron and hadron + MPI level.

### 18.43 Multi-jet observables

In observables including at least two jets, consider first the case of the $H_{T}$ distribution depicted in Fig. 92 , Over the full range and obscured by large statistical fluctuations both SHERPA samples seem to follow the NLO prediction from BlackHat+Sherpa. The LO result from GoSam+Sherpa, on the other hand, appears to fall off at the hard end of the distribution. The prediction from HEJ is a bit more subtle to judge: at low $H_{T}$ (around 100 GeV ), we see that it is in good agreement with the predictions from the other approaches. However, as higher values of $H_{T}$ are probed, the Hes prediction becomes noticeably larger than the fixed-order descriptions, including those from SHERPA where different multiplicities are merged. This is the region in $H_{T}$ where we would expect high multiplicities to have a noticeable effect, and therefore where we would expect to see the impact of the resummation in Hej. This is, however, slighlty at odds with the fact that the SHERPA prediction included up to 6 jets and that the multijet rates and the $p_{\perp}$ distributions of the fifth and sixth jet from HeJ undershoot those from SHERPA, cf. Fig. 93


Fig. 92: $H_{T}=\sum_{i \in\{\mathrm{jets}\}} E_{\perp i}$ of events with at least 2 jets on all levels of the simulation (for exact definitions and cuts see App. 18.61 and App. 18.62. Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).
and Fig. 95. However, a similar trend concerning the hard tail of this distribution appears also on the shower level in the MadGraph+Pythia sample, which includes up to 4 extra jets, and in the Powheg Box + PYthia8 sample, which includes 2 jets at LO and 1 jet at NLO. The trend is even more pronounced with an even harder tail for the PYTHIA8 MEPS sample, which includes 3 extra jets. At this level, SHERPA more or less follows the NLO result. It should be noted, though, that all approaches remain within the scale variation band indicated on the BlackHat prediction. This findings are consistently carried over to the hadron and hadron+MPI level.

Turning to the $n$-jet rates, at the matrix element level, SHERPA follows fairly closely the NLO results in different jet multiplicity bins, while HeJ seem to overshoot the central value in the 3-and 4-jet bin, but staying inside the NLO scale uncertainty band. going back to the tree-level result of SHERPA in the 5- and 6-jet bins. As discussed in Sec. 18.33, the HeJ framework includes tree-level matching for final states with up to and including four jets in the final state. Therefore it is fair to assume that the absence of matching for five jets and above leads to the larger drop in cross section observed in Fig. 93 from four-jet to five-jet as compared to that from either three-jet to four-jet or from five-jet to six-jet and lends support to the suspicion that in HEJ a matched sample would also provide larger 5- and 6-jet multiplicities. At the shower level, the trend already visible at the $H_{T}$ distribution repeats itself. The smaller cross section in the PYTHIA8 MEPS sample is mainly due to the low multiplicity bins, such that the shape of the $n$-jet distribution also has a relatively harder tail than the SHERPA sample. In contrast,


Fig. 93: Number of jets on all levels of the simulation (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that Powheg Box+Pythia8 and GoSam calculate $W+1$ jet on matrix element level, while Hej starts with $W+2$ jets and that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).
the Powheg Box +Pythia8 result, starting consistently at 1 jet, appear to be at the upper end of the NLO uncertanities throughout.

Looking at the correlation of the two leading jets in Fig. 94 at the matrix element only, both the $\Delta R$ and the $m_{12}$ distribution provided by SHERPA have a slight tilt against the NLO prediction from BLACKHAT+ SHERPA, undershooting the latter result by up to about $40 \%$ for large $\Delta R$ and by up to about $20 \%$ for large $m_{12}$. While HEJ seems to roughly follow the shape of SHERPA for $\Delta R$, it is significantly harder than SHERPA and the NLO result for large values of $m_{12}$. In addition, in both cases, HeJ also predicts a larger cross section that the other tools.

Fig. 95 shows the transverse momentum distributions for the third to sixth jets ordered in $p_{\perp}$, and at the matrix element level. For the third hardest jet, the prediction from HEJ is similar in shape but higher in cross section than the results obtained at NLO from BLACKHAT+SHERPA or the two SHERPA samples. For the fourth jet, the Hej cross section still seems higher than the other ones, but this discrepancy seems to be mainly around comparably low jet $p_{\perp}$. For larger values of $p_{\perp}$ all tree-level type or resummed predictions are below the NLO result. Surprisingly, for the fifth and sixth hardest jets, the HEJ predictions follow the SHERPA ones for low values of $p_{\perp}$ below about 60 GeV , before they fall off nearly instantly. This again may be an artefact of tree-level matching not being included in HeJ for the production of fiveand six-jets or of missing statistical support in this region of phase space.


Fig. 94: $\Delta R$ of two leading jets (left) and invariant mass of two hardest jets (right) matrix element level (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, Pythia8 and MadGraph+Pythia CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BLACKHAT+SHERPA (on matrix element level).


Fig. 95: Transverse momentum of third to sixth hardest jet on matrix element level (for exact definitions and cuts see App. 18.61 and App. 18.62). Note that BlackHat uses the CTEQ6.6 pdf, PYTHIA8 and MadGraph+PyTHIA CTEQ6L1 and all the others use CT10. In both ratio plots the ratio is taken with respect to BlackHat+Sherpa (on matrix element level).

### 18.5 Conclusions

In this study first steps towards an update and extension of the comparison in [439] have been made. In contrast to the older study, a larger variety of tools including fixed-order and resummation tools as well as NLO matched and tree-level merged simulations have been included. Not surprisingly, some observables appear to be described fairly consistently between different tools, while others exhibit large deviations, sometimes clearly beyond the formal accuracy claimed by the different methods, and also beyond the best estimates of intrinsic modelling or calculational uncertainties provided by the authors. In some instances the relative differences are way beyond naïve expectations by most of the authors of this study. This clearly hints at the need to carefully cross-validate different tools before deploying them for large scale simulations, and it also necessitates an increased collaboration of the authors of such tools in order to arrive at a more consistent picture.

We hope that this study triggered some future work towards the latter goal.

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### 18.6 Cuts and observables

### 18.61 Cuts

|  | ATLAS | CMS |
| :--- | :--- | :--- |
| lepton $p_{\perp}$ | $>20 \mathrm{GeV}$ | $>20 \mathrm{GeV}$ |
| lepton $\|\eta\|$ | $<2.5(e, \mu)$ | $<2.5(e), 2.1(\mu)$ |
| $\mathbb{E}_{\perp}$ | $>25 \mathrm{GeV}$ | no cut |
| $m_{\perp, W}$ | $>40 \mathrm{GeV}$ | $>20 \mathrm{GeV}$ |
| jet $p_{\perp}$ | $>25 \mathrm{GeV}$ | $>30 \mathrm{GeV}$ |
| jet $\|\eta\|$ | $<4.4$ | $<2.4$ |
| jet radius | $0.4\left(\right.$ anti- $\left.k_{\perp}\right)$ | $0.5\left(\right.$ anti- $\left.k_{\perp}\right)$ |
| lepton isolation | $<10 \%$ of lepton energy | $<10 \%$ of lepton energy |
|  | in cone with R=0.5 | in cone with R=0.5 |

Table 13: Cuts used in this study inspired by common ATLAS and CMS cuts.

Tab. 13 presents the cuts applied to define the event selection in both the ATLAS and CMS specifications.

### 18.62 Analysis procedure and definition of observables

A common analysis was implemented within the RIVET framework and used by all codes providing individual events. This analyses is carried out as defined in the following:

1. remove all neutrinos from all final states (i.e. 'all particles' from now on means 'all particles without neutrinos')
2. find hardest isolated lepton (electron or muon) ('lepton' from now on means 'hardest isolated lepton')
3. cut on lepton $p_{\perp}$ and $|\eta|$
4. compute missing transverse energy $E_{\perp}$ :
(a) sum the three-momenta of all particles within $|\eta|<10$, this yields $-\not p$
(b) compute missing energy as $\notin=|\boldsymbol{p}|$
(c) assume resulting four-vector $\not p$ corresponds to neutrino
5. for ATLAS cut on $E_{\perp}$
6. resonstruct $W$ four-momentum as $p^{W}=p^{\text {lepton }}+\not p$
7. compute $W$ transverse mass squared as $m_{\perp, W}^{2}=\left(p_{\perp}^{\text {lepton }}+\not p_{\perp}\right)^{2}-\left(p_{\perp}^{W}\right)^{2}$
8. cut on $W$ transverse mass
9. remove lepton from final state
10. cluster into jets keeping only those passing the $p_{\perp}$ and $|\eta|$ cuts
11. compute $H_{T}=\sum_{i \in\{\text { jets }\}} E_{\perp i}$
12. compute beam thrust $\tau_{B}=\sum_{i \in\{\text { particles }\}}\left(E_{i}-\left|p_{i}^{z}\right|\right)$ using all visible particles

It should be noted that this defintion of the $W$ is infra-red safe only for transverse observables.

### 18.7 Detailed settings

### 18.71 Sherpa

For this study Sherpa-1.3.1 was used. Except for the underlying event, which was tuned for the CT10 [255] parton distribution functions and whose parameters are given below, all other nonperturbative parameters were kept at their default values. The underlying model was tuned for the cluster hadronisation.

| K_PERP_MEAN_1 | 1.17 |
| :--- | :--- |
| K_PERP_MEAN_2 | 1.17 |
| K_PERP_SIGMA_1 | 0.760 |
| K PERP_SIGMA_2 | 0.760 |
| PROFILE_PARAMETERS | $0.576,0.353$ |
| RESCALE_EXPONENT | 0.238 |
| SCALE_MIN | 2.52 |
| SIGMA_ND_FACTOR | 0.465 |

### 18.72 Pythia8

To produce the results, we have used two tunes of Pythia8, Tune 4C and Tune A2, both of which use CTEQ6L1 parton distributions. Tune 4C is the default tune in PYTHIA8- no additional input settings are necessary. For completeness, below we list all parameters that are implicitly set by choosing the default Tune 4C.

```
PDF:pSet = 8
SigmaProcess:alphaSvalue = 0.135
SigmaDiffractive:dampen = on
SigmaDiffractive:maxXB = 65.0
SigmaDiffractive:maxAX = 65.0
SigmaDiffractive:maxXX = 65.0
```

```
TimeShower:dampenBeamRecoil = on
TimeShower:phiPolAsym = on
SpaceShower:alphaSvalue = 0.137
SpaceShower:samePTasMPI = false
SpaceShower:pT0Ref = 2.0
SpaceShower:ecmRef = 1800.0
SpaceShower:ecmPow = 0.0
SpaceShower:rapidityOrder = on
SpaceShower:phiPolAsym = on
SpaceShower:phiIntAsym = on
MultipartonInteractions:alphaSvalue = 0.135
MultipartonInteractions:pT0Ref = 2.085
MultipartonInteractions:ecmRef = 1800.
MultipartonInteractions:ecmPow = 0.19
MultipartonInteractions:bProfile = 3
MultipartonInteractions:expPow = 2.0
BeamRemnants:primordialKTsoft = 0.5
BeamRemnants:primordialKThard = 2.0
BeamRemnants:halfScaleForKT = 1.0
BeamRemnants:halfMassForKT = 1.0
BeamRemnants:reconnectRange = 1.5
```

A detailed discussion of these choices can be found in [455]. All other parameters remain with their default values. For our purposes, it might be interesting to remark that the starting value for $\alpha_{s}$-evolution in time-like splittings is given by

SpaceShower:alphaSvalue $=0.1383$
To investigate the impact of rapidity ordering in space-like showers, we chose to remove enforced rapidity ordering by setting

SpaceShower:rapidityOrder = off
If rapidity ordering is enforced in ISR, the question arises how it should be treated when picking histories. For this purpose, PYTHIA8 supplies the switch

Merging:enforceStrongOrdering
When switched "on", this parameter will result in picking non-rapidity-ordered histories only if no rapidity-ordered paths where found, thus disfavouring non-rapidity-ordered parton shower histories for matrix element states. To have a more complete understanding of the impact of tuning, we also changed to the recently proposed Tune A2 [458]. For this, we have to set

Tune:pp $=7$
Pythia8 will then reset the following parameters:

```
PDF:pSet = 8
SigmaProcess:alphaSvalue = 0.135
SigmaDiffractive:dampen = on
SigmaDiffractive:maxXB = 65.0
SigmaDiffractive:maxAX = 65.0
```

```
SigmaDiffractive:maxXX = 65.0
TimeShower:dampenBeamRecoil = on
TimeShower:phiPolAsym = on
SpaceShower:alphaSvalue = 0.137
SpaceShower:samePTasMPI = false
SpaceShower:pT0Ref = 2.0
SpaceShower:ecmRef = 1800.0
SpaceShower:ecmPow = 0.0
SpaceShower:rapidityOrder = false
SpaceShower:phiPolAsym = on
SpaceShower:phiIntAsym = on
MultipartonInteractions:alphaSvalue = 0.135
MultipartonInteractions:pTORef = 2.18
MultipartonInteractions:ecmRef = 1800.
MultipartonInteractions:ecmPow = 0.22
MultipartonInteractions:bProfile = 4
MultipartonInteractions:a1 = 0.06
BeamRemnants:primordialKTsoft = 0.5
BeamRemnants:primordialKThard = 2.0
BeamRemnants:halfScaleForKT = 1.0
BeamRemnants:halfMassForKT = 1.0
BeamRemnants:reconnectRange = 1.55
```

Apart from not enforcing rapidity ordering in space-like splittings, this tune differs from Tune 4C in that the proton size is considered $x$-dependent. This is in the spirit of Tune $4 C X$, which was introduced in [470]. In general, since we include matrix element states for two and three jets, we do not apply additional matrix element corrections in PYTHIA8 after the first emission, by setting

```
SpaceShower:MEafterFirst = off
TimeShower:MEafterFirst = off
```


### 18.73 Powheg Box + PYtHiA8

For this study we used Powheg Box rev1282 and Pythia 8.153. Except for the specific subprocess requested, the parton distribution functions set and the renormalisation/factorisation scale factors chosen, all the other parameters were kept fixed below during all the runs. Here is a sample Powheg Box input file:

```
! W^+ + jet production parameter
idvecbos 24 ! PDG id of vector boson (24: W+, -24: W-)
vdecaymode 1 ! decay channel (1: electron, 2: muon, 3: tau)
numevts 4000000 ! number of events to be generated
ih1 1 ! hadron 1 (1 for protons, -1 for antiprotons)
ih2 1 ! hadron 2 (1 for protons, -1 for antiprotons)
ebeam1 3500d0 ! energy of beam 1 in GeV
ebeam2 3500d0 ! energy of beam 2 in GeV
lhans1 192800 ! pdf set for hadron 1 (LHA numbering)
lhans2 192800 ! pdf set for hadron 2 (LHA numbering)
ncall1 100000 ! number of calls for initializing the ...
itmx1 5 ! number of iterations for initializing the ...
ncall2 250000 ! number of calls for computing the integral ...
```

| itmx2 | 4 | ! number of iterations for computing the ... |
| :--- | :--- | :--- | :--- |
| foldcsi | 1 | ! number of folds on csi integration |

When interfacing to Pythia8 we have changed the following settings with respect to Pythia8 defaults, for the various stages under investigations:
///Hadron Level w MPI and QED
BeamRemnants:reconnectRange $=1.50000$
MultipleInteractions:alphaSvalue $=0.13500$
MultipleInteractions:bProfile = 3
MultipleInteractions:ecmPow $=0.1900$
MultipleInteractions:expPow $=2.0000$
MultipleInteractions:pT0Ref $=2.0850$
PDF:pSet $=8$
SigmaDiffractive:dampen $=$ on
SigmaDiffractive:maxAX $=65.0000$
SigmaDiffractive:maxXB $=65.0000$
SigmaDiffractive:maxXX $=65.0000$
SigmaProcess:alphaSvalue $=0.13500$
SpaceShower:MEafterFirst $=$ off
SpaceShower:MEcorrections = off
SpaceShower:pTmaxMatch $=0$
SpaceShower:rapidityOrder = on
TimeShower:MEcorrections $=$ off
TimeShower:MEafterFirst $=$ off
TimeShower:pTmaxMatch $=0$
//Hadron Level w MPI (added)
SpaceShower:QEDshowerByQ = off
SpaceShower:QEDshowerByL = off
TimeShower:QEDshowerByQ $=$ off
TimeShower:QEDshowerByL $=$ off
//Hadron Level w/o MPI (added)
PartonLevel:MI = off

```
//Shower Level (added)
HadronLevel:All = off
//Parton Level (added)
PartonLevel:ISR = off
PartonLevel:FSR = off
PartonLevel:Remnants = on
```

and, most important, we have vetoed shower emissions with a transverse momentum greater than the value of SCALUP read from the Les Houches event file for the corresponding event.

### 18.74 MADGRAPH + PYTHIA

For this study MADGRAPH/MADEVENT 5.1.1.0 and Pythia 6.4.2.4 is used. The LHE files are generated for events with a $W$ and up to four additional partons, i.e. for the process:

```
pp>w- -> l-vl~ ; l-vl~~j ; l-vl~~jj ;l-vl~~jjj ; l-vl~~jjjj ;
l-vl~ ; l-vl~j ; l-vl~jj ;
l-vl~jjj ; l-vl~ jjjj ()
```

The mass of the b quark is set to zero. The strong constant $\alpha_{s}\left(M_{Z}^{2}\right)$ is set to 0.1300 both in the matrix element calculation and in the proton PDF, that is the CTEQ6L1.

Pythia is used for the parton shower and the hadronisation with the following parameters modified according to tune Z 2 .

```
MSTU(21)=1 ! Check on possible errors during program execution
MSTJ(22)=2 ! Decay those unstable particles
PARJ (71)=10 . ! for which ctau 10 mm
MSTP(33)=0 ! no K factors in hard cross sections
MSTP(2)=1 ! which order running alphaS
MSTP(51)=10042 ! structure function chosen (external PDF CTEQ6L1)
MSTP(52)=2 ! work with LHAPDF
PARP(82)=1.832 ! pt cutoff for multiparton interactions
PARP(89)=1800. ! sqrts for which PARP82 is set
PARP(90)=0.275 ! Multiple interactions: rescaling power
MSTP(95)=6 ! CR (color reconnection parameters)
PARP (77)=1.016 ! CR
PARP (78)=0.538 ! CR
PARP (80)=0.1 ! Prob. colored parton from BBR
PARP(83)=0.356 ! Multiple interactions: matter distribution para...
PARP(84)=0.651 ! Multiple interactions: matter distribution para...
PARP (62)=1.025 ! ISR cutoff
MSTP(91)=1 ! Gaussian primordial kT
PARP(93)=10.0 ! primordial kT-max
MSTP(81)=21 ! multiple parton interactions 1 is Pythia default
MSTP (82)=4 ! Defines the multi-parton model
PMAS (5,1)=4.8 ! b quark mass
PMAS (6,1)=172.5 ! t quark mass
MSTJ(1)=1 ! Fragmentation/hadronization on
MSTP(61)=1 ! Parton showering on
```

For additional studies, we set

```
MSTJ(41)=3 ! switch off lepton FSR
MSTP(81)=20 ! switch off MPI
MSTJ(1)=0 ! Fragmentation/hadronization off
```

to switch off, respectively, final state QED radiation, multi-particle interactions, and hadronisation.

## Part V

## EXPERIMENTAL DEFINITIONS AND CORRECTIONS

## 19. PHOTON ISOLATION AND FRAGMENTATION CONTRIBUTION ${ }^{43}$


#### Abstract

Photon isolation and its link with the fragmentation contribution is explored via NLO matrix-element generator and parton-shower Monte-Carlo.

Firstly the dependence of the inclusive photon and di-photon NLO cross sections to the choice of isolation criteria are investigated. The isolation criteria used is the discretized version of the Frixione isolation, with parameters chosen for those most practical at an experimental level. As an extention, a more generalized version of the standard Frixione isolation is also studied. The selection of scale is also investigated in search of the 'saddle point', which would give the optimal scale choice. In addition the choice of jet algorithm is investigated for the photon with associated jet cross section. Secondly, properties of the fragmentation contribution in parton-shower Monte-Carlos are investigated. The distance profile of the photon to the other generator level particles in the event is explored in the case of neutral mesons, fragmentation photons and direct photons. Next the impact of a "hollow" or "crown" isolation criterion, expected to enhance the fragmentation contribution, is explored. Then, to complement the NLO inclusive studies, the impact of typical Frixione isolation criteria on the fragmentation component are investigated in the parton-shower Monte-Carlos.


Finally conclusions are made comparing the properties of the fragmentation contribution in NLO generators and parton-shower generators.

### 19.1 INTRODUCTION

Experimental measurements of single photons and di-photons require the application of isolation cuts to reduce the copious backgrounds arising from jet fragmentation. Such cuts also have the impact of reducing the fragmentation contributions of photon production. On the theoretical side, including fragmentation contributions of photon production can greatly increase the complexity of the calculations, while the application of appropriate isolation cuts can effectively remove those fragmentation contributions.

[^228]
### 19.11 Frixione isolation

In the following we will study the Frixione isolation criterion [471], which was designed to suppress the fragmentation contribution. It has been shown to reduce the fragmentation contribution in NLO generators [18]. The question is to know whether or not the behavior is still applicable using parton shower Monte-Carlo and if it can be used experimentally.

We consider the following function for the isolation criterion :

$$
\begin{equation*}
E_{T}^{i s o}(R)<f(R)=\epsilon \cdot p_{T, \gamma} \cdot\left(\frac{1-\cos (R)}{1-\cos \left(R_{0}\right)}\right)^{n} \tag{19.1.1}
\end{equation*}
$$

where $E_{T}^{i s o}(R)$ is the isolation sum of all particles inside a cone of $R=\sqrt{\Delta \phi^{2}+\Delta \eta^{2}}$ around the photon, $\epsilon$ is the strength or the scale of the isolation criterion, $p_{T, \gamma}$ is the transverse energy of the photon, $R_{0}$ is the first considered cone and $n$ the power of the isolation criterion. This formula can be altered by replacing $p_{T, \gamma}$ with a fixed threshold. Functional forms $f(R)$ for different $\epsilon$ and $n$ are shown Fig. 96


Fig. 96: Examples of Frixione functional form for different parameters.

The Frixione isolation is tighter and tighter when decreasing the $R$ cone size. With matrix element NLO generators (as in Jetphox [472, 473] and Diphox [474]), the only contribution possible at a given $R \neq 0$ is the one coming from the suplementary hard jets in the event, while the fragmentation debris are emitted colinearly to the photon at $R=0$ (angle information is lost due to the fragmentation function which is integrated over the angle). With parton-shower generator, fragmentation photons are emitted off quarks at a non-zero angle during the showering process. In the following sections we will study the link between isolation and fragmentation in NLO generators, then with parton-shower Monte-Carlo.

### 19.12 Experimental complications

There are various mismatches between isolation cuts applied to theoretical calculations and isolation cuts applied to data (or to Monte Carlo). First of all, we wish to apply the isolation cut only to energy related to the hard scatter. Experimentally, most of the energy inside an isolation cone is due to the underlying event associated with the hard scatter, or the remnants of additional interactions in the same crossing. Techniques such as jet area subtraction [475, 476] can be used to remove an amount of energy from the isolation cone roughly equal to the expected contamination from underlying event/pileup, leaving only energy related to the hard scatter and specifically to fragmentation processes. Since there is no underlying event/pileup in partonic level theory calculations, only the isolation cut needs to be applied to the theory.

Full details of the use of this correction within the ATLAS collaboration can be found in the inclusive cross section measurement [477]. The ATLAS isolation definition uses a cone around the cluster of cells that are identified as a photon. These photon cluster cells are not included in the sum, so there is first a correction for any leakage of the photon shower into the surrounding cells (typically a few percent of the photon $p_{T}$ ). The pile-up/underlying event correction is then applied by calculating per event the ambient energy from the jet activity in that specific event. This follows the jet area corrections method mentioned above, where all jets are reconstructed without any minimum momentum threshold. The energy density of each jet is calculated and the median density is used for the correction. In 2010 this typically resulted in a correction of around 900 MeV .

The original Frixione isolation scheme assumed that an isolation cut could be applied continuously as a function of R (distance from the photon). Actual detectors have a finite granularity. A solution to this was the adoption of a discretized version of Frixione isolation, allowing this granularity to be taken into account [18]. However, it is not possible to place an isolation cut on the inner-most cone (typically $R \sim 0.1$ ), because of the presence of the photon itself. While the separation between the fragmentation photon and the jet remnants is finite in data (and in Monte Carlo), fragmentation is treated as a collinear process in partonic cross sections. The inability to apply the isolation cut down to $R=0$, results in a greatly reduced ability to discriminate against fragmentation processes in the partonic level theory.

To rectify this the Frixione calculation could be modified into a 'crown' isolation, whereby the last cone is missed from the calculation. Unfortunately as most of the radiation is collinear in the fragmentation events, it is likely to reduce its effect of removing these events. Other studies [478] have shown that the photon quality cuts applied by the experiments will reduce the fraction of fragmentation photons accepted, where substantial fragmentation energy is collinear with the photon. However, the rejection is not $100 \%$, so we are still left with a smaller reduction of fragmentation contributions in the partonic level theory than are actually (presumably) present in the data. In these proceedings, we will discuss how to more properly incorporate the correct level of rejection in the theory.

### 19.13 Choice of fragmentation scale

In addition to the experimental difficulties with applying the isolation criteria there are also difficulties in choosing appropriate scales for the theoretical calculation. This is discussed in the following text, along with other considerations for applying Frixione isolation at a theoretical level.

Fragmentation is treated as a collinear process in partonic calculations. In this framework, the original "continuous" Frixione criterion [471] was designed to inhibit the appearance of final state photonparton collinear singularities which otherwise require absorption in a fragmentation function $D\left(z, M_{F}\right)$. Thus, cross sections for the production of prompt photons isolated with this criterion involve no fragmentation contribution. Discretized variants of this criterion have been proposed which aim at matching better what can be actually implemented experimentally [18]. They consist in a limited number of nested cones $\mathcal{C}_{j=1, \cdots, n}$ with respective radii $R_{1}=R_{\min }<R_{2}<\cdots<R_{n}=R_{\max }$ defined in the azimuthal and rapidity differences with respect to the photon direction, and requiring recursively that the accompanying hadronic transverse energies inside every successive cone $\mathcal{C}_{j}$ be less than an ordered sequence of maximum values ${ }^{44} E_{T j}^{i s o}$ such that $0<E_{T 1}^{i s o}<\cdots<E_{T n}^{i s o}$. However, in contrast with the continuous criterion, such discretized variants still involve a fragmentation contribution, though the latter is expected to be small, since the situation in the innermost cone shares some similarity with the standard cone criterion. When quantifying the magnitude of the fragmentation contribution with such discretized criteria, a potentially tricky issue concerns the fragmentation scale dependence and the "best choice" of scale.

This issue matters for isolation with the standard cone criterion when the radius $R$ of the cone is $\ll 1$ while $E_{T}^{i s o}$ is kept fixed. Whereas the natural fragmentation scale $M_{F}$ in the non-isolated case

[^229]is $\sim p_{T}^{\gamma}$, this choice can lead to very poor theoretical estimates at Next to Leading Order (NLO) in perturbative QCD when $R \ll 1$ [472]. The scale dependence near the choice $M_{F} \sim p_{T}^{\gamma}$ is then large and, worse, the theoretical prediction may eventually exhibit an unphysical violation of unitarity whereby the predicted NLO cross section for photons becomes larger than the inclusive one, so that even for only moderately small $R$ the reliability of the prediction is questionable. On the other hand, as ${ }^{45} D\left(z, M_{F}\right) \sim$ $\log \left(M_{F} / \Lambda_{Q C D}\right)$, with the choice $M_{F} \sim R p_{T}^{\gamma}$ the fragmentation contribution is suppressed compared with $M_{F} \sim p_{T}^{\gamma}$. The situation is improved regarding both scale dependence and unitarity, although it does not solve the problem completely. One actually faces a multiscale problem: $\Lambda_{Q C D} \ll R p_{T}^{\gamma} \ll p_{T}^{\gamma}$, and a one-scale compromise is possibly insufficient depending on the kinematical regime explored. The atypical choice $M_{F} \sim R p_{T}^{\gamma}$ has in principle to be supplemented by a resummation of the logarithmic $R$ dependence coming form outside the cone, if at all possible. At leading-log $R$ (LLR) accuracy at least, such a resummation is actually feasible, which furthermore allows to solve the apparent puzzle why scale choices should be very different in the cases with isolation in a narrow cone vs. broad cone or without isolation.

The concern about the discretized Frixione criteria is that the innermost cone size is quite small. The choice for the fragmentation scale $M_{F}$ shall then arguably be $M_{F} \sim \mathcal{O}\left(R_{\min } p_{T}^{\gamma}\right)$. On the other hand, as the allowed transverse energy deposit $E_{T}^{i s o}\left(R_{\text {min }}\right)$ inside this cone is correspondingly small, the width of the interval in the fragmentation variable on which the fragmentation function is convoluted with the partonic cross section is restricted to a rather narrow range $0<1-z<E_{T}^{i s o}\left(R_{\min }\right) / p_{T}^{\gamma} \sim$ $\epsilon\left(R_{\min } / R_{\max }\right)^{n}$. This leads to a quite suppressed fragmentation contribution. The combination of the two effects: a low fragmentation scale and a narrow $z$-range, is the discrete counterpart of the inhibition of fragmentation by the continuous criterion. We may thus expect that the issue of the narrow cone is less worrying for the reliability of the NLO calculation in this case than if only $R$ were taken small while keeping $E_{T}^{i s o}$ fixed. In order to assess the uncertainty on the fragmentation contribution we may perform the calculation for the "arguably better" scale $M_{F} \sim R_{\min } p_{T}^{\gamma}$ and compare it to the expectedly larger result for the standard choice $M_{F} \sim p_{T}^{\gamma} / 2$.

### 19.2 ISOLATION FOR INCLUSIVE PHOTONS AND DIPHOTONS AT NLO

The study at NLO uses the Jetphox generator to calculate the inclusive photon cross section and Diphox for the di-photon cross section. Details of how to use the software and to obtain predictions with errors can be found in [480] and the selection criteria used are listed in the appendix. Previous results from Les Houches [18] showed that the discretized Frixione isolation criteria did manage to reduce the fragmentation contribution, here we extend that study in several ways. Firstly the cross section returned has been compared to that calculated from using the standard cone isolation, as used in current measurements. A generalized form of the Frixione isolation is discussed, aimed to satisfy both the experimental and the theoretical requirements on the isolation cut for different $p_{T}$ regimes. In addition the effects of changing the number of cones used in the calculation and of choosing an $E_{T}$ cut, rather than relating it to the photon $p_{T}$, are investigated. In addition, further complications to comparing theoretical and experimental isolation calculations are discussed. Finally there are further brief studies using Jetphox to look at scale and jet algorithm choices.

### 19.21 Discretized prescription

The parameters used to define different selections, according to Eq. 19.1.1, were:

$$
\begin{array}{llll}
a: \epsilon=0.05 n=0.2 & b: \epsilon=1 n=0.2 & c: \epsilon=1 n=1 & d: \epsilon=0.5 n=1 \\
e: \epsilon=0.05 n=1 & f: \epsilon=1 n=0.1 & g: \epsilon=1 n=0.5 &
\end{array}
$$

[^230]

Fig. 97: Left: Fragmentation fraction for the cone and Frixione isolation criteria. Right: The applied $E_{T}$ cut on the isolation sum as a function of $p_{T}$ for the 0.4 cone or 0.1 cone in the Frixione criteria.
where all but the last two were based on the previous study. In all cases $R_{0}$ was chosen to be 0.4 , with $R$ being set to either: $0.4,0.3,0.2,0.1$ or $0.4,0.35,0.3,0.25,0.2,0.15,0.1$.

The comparison to the cone isolation in Fig. 97 shows that out of the chosen parameters only 1 set removes the fragmentation contribution more than what is removed by the cone algorithm, although two are lower until high $p_{T}$. It also shows that criteria $b$ and $f$ are not much better than applying no isolation criteria at all. When altering Eq. 19.1 .1 to use a fixed $E_{T}=4 \mathrm{GeV}$ instead of $p_{T, \gamma}$ the results are more promising but this is because it applies a cut in the 0.1 cone that is below the experimental accuracy (of the order 100 MeV due to detector resolution/noise). Unfortunately Fig. 97 also shows that this is also the case for the $p_{T}$ requirements, as case $e$ (the only criteria to perform better than the standard cone) also applies a cut that is not viable experimentally in the 0.1 cone.

There are some positive outcomes from these studies, firstly the Frixione criteria $b$ and $d$ maybe useful criteria to use experimentally as they keep the fragmentation contribution similar and low in all bins, which could help with understanding of the systematic errors/correlation between bins. Secondly the comparison of the number of cones used in the Frixione criteria resulted in a difference of around $1 \%$ on the total cross section and almost no effect on the fragmentation fraction. This means that it is fine to use the lower number of cones case, and that the discrete Frixione criteria is most likely very similar to that of the continuous version.

### 19.22 Generalized prescription

As seen previously, to remove the fragmentation contribution in the theory, a small value of $\varepsilon$ is needed. However, given the effects of finite resolution and granularity on the experimental description of the isolation energy, a minimum threshold has to be allowed in the isolation cone, especially at low $p_{T}$. A typical value of $2-4 \mathrm{GeV}$ is used as experimental cut, to optimize the rejection of hadronic background coming from the decay of light mesons. Now, at high $p_{T}$ this cut might result too tight, particularly on the theoretical side given that an isolation cut much smaller than the photon $p_{T}$ can cause large logs in the calculations, this effect was not observed in the previous Les Houches study.

As a good compromise of these two requirements, it has been proposed [481] to extend the original


Fig. 98: Effect of the two terms in the modified Frixione isolation prescription effects of the different pieces of the generalized Frixione isolation prescription on the isolation cut as a function of $p_{T}$ (left) and the cone radius R (right).

Frixione prescription (Eq. 19.1.1) to a more general form:

$$
\begin{equation*}
E_{T}^{i s o}<\left(\left(E_{0}\right)^{k}+\left(\varepsilon \cdot p_{T}\right)^{k}\right)^{1 / k}\left(\frac{1-\cos R}{1-\cos R_{0}}\right)^{n} \tag{19.2.1}
\end{equation*}
$$

where:
$R_{0}$ is the maximum cone size
$E_{0}$ is the minimum energy pedestal allowed in a cone of size $R_{0}$
$\varepsilon$ is the fraction of the photon $p_{T}$ allowed in the cone of size $R_{0}$
$k$ determines the shape of the isolation profile in $p_{T}$
$n$ determines the shape of the isolation profile in R (see Fig. 98 right])
The extra parameters give enough flexibility to ensure a (finite) tight cut at low $p_{T}\left(\sim E_{0}\right)$ and, at the same time, a loose cut at high end of the spectrum driven by the photon $p_{T}$. The $k$ parameter controls how quickly/smoothly is the transition from one regime to the other (see Fig. 98 left]).

This generalized prescriptior ${ }^{[46}$ has been implemented in Jetphox recently and some possible configurations are explored here. The studied configurations vary $\varepsilon(=0.05,1)$ and $k(=2,5,10)$, and have a fixed value for $E_{0}=4 \mathrm{GeV}$ (the typical cut applied in ATLAS) and $n=0.5$ (given the linear behaviour of isolation distribution width observed for direct photons in ATLAS [482]).

The high- $\varepsilon$ configurations ( $\varepsilon=1$ ), show a worse performance at removing the fragmentation contribution with respect to the fixed cone approach and are practically insensitive to the value of $k$ in the formula. The remaining fragmentation fraction is $\sim 25 \%$ at 45 GeV decreasing to $20 \%$ in the highest $p_{T}$ bin. On the other hand, as seen in Fig. 99, all the configurations for a low value of $\varepsilon(=0.05)$ show an improvement in fragmentation rejection compared to both the no isolation and fixed cone cases, in the whole $p_{T}$ region ( $45 \mathrm{GeV}<\mathrm{p}_{\mathrm{T}}<600 \mathrm{GeV}$ ). The $p_{T}$ profile for the smaller cone ( $R=0.1$ ) in this case (Fig. 99[right]) looks also more promising in terms of its applicability at the experimental level.

[^231]

Fig. 99: Left: Fragmentation fraction for the cone and the (generalized) Frixione isolation criteria. Right: The applied isolation cut as a function of $p_{T}$ for 0.1 cone in the (generalized) Frixione criteria.

### 19.23 Continuous and discretized Frixione criteria in di-photon events

Following the previous studies with inclusive photons, we now consider the production of photon pairs. The aims of this study are i) to assess the effect on the magnitude of the fragmentation contribution by comparing results from using the continuous Frixione criterion with those using several variants of the discretized version, implemented in the NLO programme Diphox, thereby providing a NLO assessment of how much fragmentation may be missing in the NNLO calculation of Catani et al. [78] which includes no fragmentation and therefore uses the continuous criterion; ii) to probe the dependence of the prediction with respect to the fragmentation scale choice. It supplements a similar comparison which had been performed for inclusive photon production in [18].

Fig. 100 provides a comparison of the original continuous criterion to the discretized version of the criterion based on four nested cones with respective radii $R_{\text {min }}=0.1, R_{2}=0.2, R_{3}=0.3$ and $R_{\max }=0.4$. Four variants of the energy profile $E_{T}^{\text {iso }}(R)$ as defined in Eq. 19.1.1 have been considered: $(\epsilon, n)=(0.05,0.2),(0.05,1),(0.5,1)$ and $(1,1)$. Fig. 100 (left) presents the distribution in invariant mass of photon pairs in the range $40 \mathrm{GeV} \leq m_{\gamma \gamma} \leq 300 \mathrm{GeV}$. The discretized criterion $(0.05,1)$ suppresses fragmentation so much that there is practically no difference between the discretized and continuous versions. With the criterion $(1,1)$, the discretized version leads to a distribution $O(10-12 \%)$ larger than the continuous one. The choice $(0.5,1)$ displays a similar feature, though quantitatively less important. The energy profile of the fourth choice is not suited for an efficient isolation unless $\epsilon$ is chosen very small. A similar comparison is shown on Fig. 100 (right) for the distribution in the difference in azimuthal angle $\Delta \phi$ between the two photons. Whereas the distribution in invariant mass is dominated by the direct contribution, the tail of the distribution in $\Delta \phi$ tail at low $\Delta \phi$ is more sensitive to the fragmentation contribution. Therefore, the conclusions are qualitatively similar to the one drawn for the distribution in invariant mass, yet the effects are quantitatively larger.

Fig. 101 assesses the dependence on the fragmentation scale $M_{F}$, for the distributions in invariant mass (left) and in $\Delta \phi$ (right) respectively. Two choices were considered: $M_{F}=R_{\min } \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}=$ $0.1 \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}$ vs. $M_{F}=R_{\max } \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}=0.4 \min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}$ closer to a standard choice ${ }^{47}$. As expected, the distribution in invariant mass, which is not very sensitive to the fragmen-

[^232]

Fig. 100: Comparing continuous and discretized Frixione criterions for the distributions in $m_{\gamma \gamma}$ (left) and $\Delta \phi$ (right) of photon pairs, for four variants of the criterion.


Fig. 101: Fragmentation scale dependence of the distribution in $m_{\gamma \gamma}$ (left) and $\Delta \phi$ (right) of photon pairs, for four variants of the discretized Frixione criterion.
tation contribution, is practically not impacted by the choice. The distribution in $\Delta \phi$ is more sensitive to the fragmentation component and the sensitivity to the fragmentation scale choice is larger than for the distribution in invariant mass. The sensitivity to the fragmentation scale choice is the largest in the case of the criterion $(\epsilon, n)=(1,1)$, for which the predictions are $5-7 \%$ smaller, rather uniformly, with the lower scale choice than with the more standard one.

In conclusion this preliminary study shows that the impact of the fragmentation contribution passing the discretized criterion seems to be almost negligible on the distribution in invariant mass, and remains small even on the tail of the distribution in azimuthal angle. Notwithstanding, the conclusions shall have limited use depending on how isolation is actually implemented experimentally in the innermost cone. We here stick to a discretized version of the Frixione criterion which respects the original idea of a transverse energy deposit decreasing towards zero with the cone radius. If instead any experimental constraint would allow a more permissive condition in the innermost cone, a dedicated study would be mandatory.

### 19.24 Additional studies at NLO

In addition to the isolation studies with Jetphox, we present here two brief studies as an attempt to reduce the theoretical errors from the NLO calculation. These study the choice of renormalizaion and factorization scale parameter and secondly the jet algorithm parameters.

As studied in [480], the scale choice is set to a fraction of the photon $p_{T}$. By altering this fraction around the central value of 1.0 , it is hoped to gain an uncertainty on the terms missed in the NLO calculation. The best selection for this central value would be to be at a 'saddle point', where moving in any direction from this point gives similar changes in the cross section. However, it is found that as the scale is reduced (in steps: $2.0,1.0,0.5,0.25,0.1,0.05$ and 0.01 ) the cross section increases, when moving the two scales coherently or independantly. One difference in this result to the previous study was that it was carried out in three $p_{T}$ bins, but the result remained the same for all (only the highest bin was able to be calculated with a scale of 0.01 ). Similarly the addition of using Frixione isolation instead of the standard cone isolation also resulted in the same cross section behaviour. The summary of this is that there must be large contributions needed from NNLO. However, on the positive side, in all $3 p_{T}$ bins, the variation between 0.5-1.0-2.0 resulted in differences of similar magnitude around 1.0 , so this is likely a safe estimate of the uncertainty.

After the inclusive photon measurements, the next step experimentally is to require the addition of at least one jet. Using a jet of 10 GeV the cross section was calculated for two algorithms each for multiple sizes:

- Kt algorithm with $\Delta R=0.3,0.4,0.5$ or 0.6
- Cone with $\Delta R=0.4,0.5$ or 0.6

These choices had an affect of $<1 \%$ on the cross section computed in 3 photon $p_{T}$ bins, suggesting that this will not increase the error for the NLO calculation when moving from the inclusive cross section to that with an additional jet.

### 19.3 FRAGMENTATION PHOTONS IN PARTON-SHOWER MONTE-CARLO

The second part of this study continues to investigate photon isolation, but now in di-photon events using parton-shower Monte-Carlo generators; again the selection used is listed in the appendix. The study begins by investigating the distance between the photon and other particles. It then moves into studying several different styles of isolation criteria, including Frixione criteria as done in the inclusive NLO studies.
encodes the two photons in a symmetrized way.

### 19.31 Topology of fragmentation photons

We consider three sets of parton-shower Monte-Carlo samples for the $\gamma \gamma+\mathrm{X}$ process:

- Pythia [400] $\gamma \gamma$ Born and Box direct processes, plus the Pythia $\gamma+$ jet process with the jet fragmenting into a photon ( 20 million events were generated for the $\gamma+$ jet sample and 1000 times more would have been needed for the dijet fragmenting to two photons due to the low $q \rightarrow \gamma$ branching ratio for isolated photons).
- Pythia $\gamma \gamma$ Born and Box direct processes, plus the Pythia $\gamma+$ jet process with the jet fragmenting into a photon and the Pythia dijet process with the two jets fragmenting into photons. Both Pythia $\gamma+$ jet and dijet samples were generated with a filter which enhances the presence of events with isolated electromagnetic particles.
- Madgraph [165] $\gamma \gamma+$ up to two supplementary hard jets, with fragmentation/hadronization done with Pythia.
The fragmentation contribution is included as a bremsstrahlung contribution in Madgraph at matrix element level, while it is included as a showering contribution in Pythia $\gamma+$ jet and dijet (in the PYTHIA samples we identify fragmentation photons as those having a quark or gluor ${ }^{48}$ as parent). The fragmentation fraction found is compatible with ref [483]. We consider additionally the case where the two jets fragment into boosted neutral mesons ( $\pi^{0}, \eta, \rho$ and $\omega$ ) that can experimentally mimic direct or fragmentation photons at reconstructed level because of the finite granularity of the detector. These samples include an underlying event but were generated without pile-up.


Fig. 102: $\Delta R$ distance distribution between the photon and the other generator-level particle candidates in the event, for neutral mesons, fragmentation photons and partonic photons.

Fig. 102 shows the $\Delta R$ distance between the photon or neutral mesons and the other particle candidates in the event. Partonic photons, fragmentation photons and neutral mesons have different properties as a function of $\Delta R$. Partonic photons in Pythia have a linear behavior, which is expected because the only contribution that can enter in the isolation sum is the underlying event and pile-up (with also a small contribution from QCD radiation at the shower level) which is expected to be uniform in space. As each bin consists of an annulus with radius growing linearly as a function of $R$, the quantity

[^233]of particles grows linearly with $R$ in the area of the annulus. Neutral mesons have a radically different profile, with a peak of the $\Delta R$ distribution close to 0 . The peak is caused by the decay of particles resulting from jet fragmentation close to the neutral meson direction. Pythia fragmentation photons have a behavior somehow in between that of neutral mesons and partonic photons. The peak at low $\Delta R$ is still present but much reduced with respect to that of neutral mesons. Madgraph partonic photons exhibit a modulation of the Pythia partonic photon $\Delta R$ distribution, probably because Madgraph includes fragmentation as a bremsstrahlung contribution.

From this we can expect that the smaller the $\Delta R$ cone used in Frixione isolation (until $\Delta R \simeq 0.1$ ), the higher the discrimination against the neutral mesons and fragmentation photons. The discrimination against neutral mesons is higher than that against fragmentation photons (as is well-known experimentally). This can be seen in Fig. 103, which shows the isolation sum profile divided by the transverse energy of the photon for different cone sizes.


Fig. 103: Isolation sum normalized to the photon energy computed in cones of size $\Delta R<0.1$ (top left), $\Delta R<0.2$ (top right), $\Delta R<0.3$ (bottom left), $\Delta R<0.4$ (bottom right), for neutral mesons, fragmentation photons and partonic photons.

Table 14: Fraction represented by the 1-fragmentation and 2-fragmentation contributions for various Frixione isolation criteria in Pythia two-prompt photon samples (with electromagnetic enrichment filter).

| Criteria | 1-frag fraction | 2-frag fraction | 1,2-frag fraction |
| :---: | :---: | :---: | :---: |
| Solid $\Delta R<0.4, E_{T}^{\text {iso }}<5 \mathrm{GeV}$ | 0.335 | 0.157 | 0.492 |
| Hollow $0.1<\Delta R<0.4, E_{T}^{\text {iso }}<4 \mathrm{GeV}$ | 0.337 | 0.168 | 0.505 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=1.0$ | 0.322 | 0.145 | 0.467 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=0.2$ | 0.318 | 0.147 | 0.466 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.2$ | 0.372 | 0.228 | 0.599 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.1$ | 0.374 | 0.232 | 0.601 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=1.0$ | 0.353 | 0.192 | 0.545 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.5$ | 0.365 | 0.212 | 0.577 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.5, n=1.0$ | 0.343 | 0.176 | 0.518 |

### 19.32 Impact of hollow cones on the fragmentation contribution

In NLO generators, the products of the quark fragmentation are along the fragmentation photon direction. In parton-shower generators we have seen that this is not necessarily true. In NLO generators, the "hollow" or "crown" isolation, where the energy sum has to be below a fixed threshold in a region $R_{1}<\Delta R<R_{2}$ while in the region $R<R_{1}$ any arbitrary amount of energy is admitted, has been shown to enhance the fragmentation contribution with respect to the usual "solid" isolation. This "hollow" isolation is interesting also because this criterion is closer than the "solid" cone to what is used experimentally (it allows to exclude from the isolation sum the energy deposited by the photon itself). The first two lines of Tables 14 and 15 show that in general the fragmentation fraction does not increase significantly when moving from solid to hollow cone isolation, for the PYTHIA samples.

### 19.33 Impact of Frixione isolation on the fragmentation contribution

Tables 14 and 15 report the fragmentation fraction inside the Pythia two-prompt sample for different Frixione isolation criteria. Eight isolation cones were used : $\Delta R<0.05, \Delta R<0.1, \Delta R<0.15$, $\Delta R<0.2, \Delta R<0.25, \Delta R<0.3, \Delta R<0.35, \Delta R<0.4$. The results are almost identical if instead four cones are used ( $0.1,0.2,0.3,0.4$ ), as found at NLO. The tables show that in both the electromagnetically-enriched samples and non-enriched samples, the discrete Frixione isolation with the usual functional form $f(R)$ does not reduce the fragmentation contribution with respect to the standard isolation criterion (with a cone $\Delta R<0.4$ ) except when the parameter $\epsilon$ is at its smallest value, $\epsilon=$ 0.05 , for which modest reductions of between 5 and $8 \%$ can be achieved. The cause of this apparent non-optimal behavior can be explained by the non-collinearity of the fragmentation debris around the fragmentation photon in PYTHIA. Frixione isolation is designed to apply tighter and tighter isolation criteria $E_{T}^{i s o}<f(R) \rightarrow 0$ as $\Delta R \rightarrow 0$, assuming that most of the fragmentation debris are around $\Delta R \simeq 0$. As it is seemingly not the case in the parton-shower Monte-Carlo studied here, the criterion loses most of its discrimination power.

The previous study suggests that the previous working points studied with the Frixione functional form $f(R)$ might not be optimal for the rejection of fragmentation debris. In figure 104 we compare the performance of three different sets of criteria: 1) non-Frixione isolation in a single cone $\Delta R<0.4,2$ ) optimized working points for the parameters in the Frixione functional form (four cones $0.1,0.2,0.3,0.4$ were used to make the algorithm converge faster), 3) re-optimized 'Frixione' isolation criteria on cones $\Delta R<0.1,0.2,0.3,0.4$ without using the explicit functional form (we no longer constrain the events to satisfy $E_{T}^{i s o}<f(R)$ and let $f(R)$ free). In the second case, an optimization procedure is performed scanning over the parameters $\epsilon$ and $n$ to find the best working points (corresponding to a maximum

Table 15: Fraction represented by the 1 -fragmentation contribution for various Frixione isolation criteria in Pythia two-prompt photon samples (without enrichment filter).

| Criteria | 1-frag fraction |
| :---: | :---: |
| Solid $\Delta R<0.4, E_{T}^{i s o}<5 \mathrm{GeV}$ | 0.455 |
| Hollow $0.1<\Delta R<0.4, E_{T}^{i s o}<4 \mathrm{GeV}$ | 0.458 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=1.0$ | 0.420 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.05, n=0.2$ | 0.419 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.2$ | 0.514 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.1$ | 0.519 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=1.0$ | 0.489 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=1.0, n=0.5$ | 0.503 |
| Frixione 8 cones, $E_{T}=20 \mathrm{GeV}, \epsilon=0.5, n=1.0$ | 0.465 |

efficiency for a given $s / b$ ). In the last case, an optimization code is used to find the best selection criteria to be applied on $E_{T}^{i s o}$ for each $\Delta R$ cone. The optimization takes as input the target value of $s / b$ (partonic signal over fragmentation background ratio), then relaxes and tightens each cut separately with an iterative procedure to find the best signal efficiency for this $s / b$ target. The procedure was performed to find the working points corresponding to the $s / b$ obtained with the first Frixione criterion.

Figure 104 shows that the optimized working points for the Frixione functional form perform slightly better than the standard isolation for a given photon efficiency, and that optimization using no functional form in turn performs slightly better than the Frixione functional form; for the same value of single-photon efficiency, lower values of fragmentation fraction are attainable. It should be noted that this optimisation leads to a looser cut on the first cone, $\Delta R<0.1$, than the usual functional form. Nevertheless, to obtain reductions in the fragmentation fraction of more than $10 \%$, increasingly significant reductions in single photon efficiency are required, since the fragmentation reduction becomes nearly flat.

All in all, with the definition of the isolation in a cone of $\Delta R$ used here, which is a usual way of defining isolation at the experimental level (where one has however to remove the footprint of the photon from the isolation sum and to cope with pile-up), rejecting fragmentation photons can be done only at a cost of a lowered signal efficiency. With this optimization procedure it was found that to decrease the fragmentation fraction by $10 \%$, a signal loss of about $60 \%$ has to be achieved, leading to extremely tight cuts probably not applicable in experimental analysis.

## CONCLUSIONS

Firstly for the NLO cross sections, it was found that only one of the Frixione isolation criteria suggested in [18] actually performs better at removing the fragmentation contribution in the inclusive case than that of the standard cone, although potentially too tight to use experimentally. However, it is useful to see that the results are independent of the number of cones used. This is also the case for the di-photon cross section where it compares well to the continuous criteria. A more promising result in the inclusive case is that the generalized version of Frixione isolation, with small values of $\epsilon$, do significantly reduce the fragmentation fraction without applying too tight a cut in the smallest cone. In addition it is confirmed that the 'saddle point' can not be found when altering the scale choice for the inclusive cross-section, suggesting more corrections needed at NNLO. Finally when moving to the photon with associated jet cross section, from the inclusive cross section, it is reported that the jet algorithm (or size) used at NLO makes little difference to the cross section.

In the study at the parton-shower level it was shown that the isolation profile of fragmentation


Fig. 104: The fraction of the 1 -fragmentation contribution vs single $\gamma$ efficiency for various sets of criteria. Blue : tested working points reported on table 15. Black : selection criteria on isolation in $\Delta R<0.4$. Green : Optimized Frixione isolation using the usual functional form. Red : Re-optimized isolation criteria on cones $\Delta R<0.1,0.2,0.3,0.4$ without using the functional form.
photons is no longer collinear anymore, whereas the modelization of the fragmentation function in NLO generators leads the quark/gluon debris to be collinear to the photon. Furthermore, the hadronization process of the quark/gluon that emitted the photon leads to a $\Delta R$ profile which is no longer peaked at zero (but close to zero). In parton-shower programs isolation still has increasing discriminating power when going lower in $\Delta R$. However, it was found that a $10 \%$ decrease in fragmentation fraction in diphoton events with respect to standard isolation leads to a drop in single photon signal efficiency to approximately $60 \%$ of the initial value. The usual functional form for Frixione isolation was shown to be not completely optimal for suppressing the fragmentation contribution while preserving high signal efficiency. This can be mitigated by re-optimizing the cuts for each $\Delta R$ of the discrete Frixione prescription, which allows a looser cut in the innermost cone. Further studies using other fragmentation modelizations in parton-shower programs like SHERPA [427] (LO matrix-element where photons and jets in the shower are matched to matrix element level) or POWHEG [484] (NLO matrix-element with consistent fragmentation photon matching) would need to be investigated.

In conclusion the results from the two studies show there are differences and similarities at the two levels. Regarding the fragmentation fraction, this is far more reduced at the NLO level than at the parton-shower level. However, the two levels show agreement that the results from Frixione isolation are independant of the number of cones used and that similar shape cuts can be obtained by retuning cuts at the parton-shower level and by using the generalized prescription at NLO.

## ACKNOWLEDGEMENTS

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## APPENDIX: Selection details

All of the studies are carried out for $p p$ collisions at $\sqrt{S}=7 \mathrm{TeV}$. For simplicity the the inclusive studies are carried out for the region where the photon lies in $|\eta|<0.6$. When calculating the cone isolation around the photon a cone of 0.4 is used with the requirement that the energy in the cone is less than 4 GeV . The renormalization scale $\mu$ and initial state factorization scale $M$ are set to the photon $p_{T}$,
unless stated otherwise, and the CTEQ6.6 PDF[256] is used and the photon fragmentation functions are BFG set II [479]. For the generalized Frixione isolation case, the cones used are: $\mathrm{R}=0.4,0.35,0.3,0.25$, $0.2,0.15$ and 0.1.

In the NLO di-photon studies, the photons have: $p_{T}^{\gamma 1} \leq 25 \mathrm{GeV}, p_{T}^{\gamma 2} \geq 22 \mathrm{GeV}$, in the rapidity range $\left|\eta^{\gamma}\right| \leq 2.5$ for both photons, and a separation $\Delta R_{\gamma \gamma} \geq 0.4$ is required between the two photons. The mass range considered is $40 \mathrm{GeV} \leq m_{\gamma \gamma} \leq 300 \mathrm{GeV}$. In this case the scales $\mu$ and $M$ are chosen equal to $\min \left\{p_{T}^{\gamma 1}, p_{T}^{\gamma 2}\right\}$.

In the parton shower di-photon studies, the photons are selected with: $M_{\gamma \gamma}>80 \mathrm{GeV}, p_{T}>21,20$ $\mathrm{GeV},|\eta|<2.5$ and $E_{T}^{i s o}<5 \mathrm{GeV}$.

## 20. EVENT-BY-EVENT PILEUP SUBTRACTION USING JET AREAS 49


#### Abstract

In these proceedings, we compare the efficiency of several jet-area-based subtraction methods to correct for pile-up contamination at hadronic colliders. We study the dependence on various variables like the $p_{t}$ and rapidity of the jets, the number of pile-up vertices or the Monte-Carlo generator variations. We conclude that estimations of the pile-up density using a median computed over grid-cell patches, including a rescaling to correct for the rapidity dependence, perform particularly well, though alternative methods are possible.


### 20.1 Introduction

With the LHC running at larger and larger luminosities, hard $p p$ interactions are accompanied by an increasing number of pile-up (PU) collisions: from a few PU events per bunch crossing in spring 2011, operation with $\sim 20 \mathrm{PU}$ events is now routine. Considering only in-time PU , this would lead to an extra transverse momentum of $\sim 750 \mathrm{GeV}$ deposited in the event, and a jet of a typical radius $R=0.5$ would see its transverse momentum shifted by $\sim 10 \mathrm{GeV}$. In order to obtain a good energy resolution for the jets it is therefore mandatory to correct for this contamination.

In these proceedings, we review several methods - both existing methods and new refinements - to subtract the contamination due to PU and provide a systematic study of their efficiency.

It is important to note already now that PU has not only the effect to shift the momentum of the jets: it also smears their momentum. Indeed, the number of PU vertices varies from one collision to the next (following a Poisson distribution varying with the beam conditions), all PU interactions, i.e. minimum bias collisions, do not lead to the same energy deposit, and finally, the energy produced in a minimum bias collision is not deposited uniformly across the detector. Altogether, on top of an average shift, PU will add two sources of resolution smearing: event-to-event and in-event fluctuations corresponding respectively to variations of the PU activity from one event to another and from one point to another in a single event.

Here we shall primarily study in-time $P U$, that is the effects coming from multiple $p p$ interactions that occur in the same bunch crossing as the hard interaction one triggers on. Because of the response time inherent to each detector this would come with a second effect, out-of-time $P U$, corresponding to the PU activity in the few bunch crossings preceding the one with the hard interaction. Since these heavily depend on the details of each individual detector - and even varies from one sub-detector to another - it goes beyond the scope of this theoretical study. However, as we shall discuss in further detail later on, the PU subtraction methods proposed here do not make any assumption about a distinction between in-time and out-of-time PU and thus should be robust enough in more complex cases.

[^234]
### 20.2 Subtraction method(s)

We are interested in the situation where a hard event is contaminated by a background coming from additional pileup interactions. A reconstructed jet in that full event (hard event + background), which we shall call a full jet, differs from the hard jet in the original hard event because of the presence of the background. By background subtraction, we mean correcting the full jet in such as to recover the momentum of the original hard jet, i.e. subtract the pileup contamination from the jet's momentum.

### 20.21 Background effects

Our starting point is to realise [485] that a uniform background affects the momentum of a jet in two ways: it shifts its momentum because of the background particles clustered with the jet, and it modifies the way the hard particles themselves are clustered because the background particles are not infinitely soft.

This means that the reconstructed momentum has the form 50

$$
\begin{equation*}
p_{t, \text { full }}=p_{t, \text { hard }}+\rho A \pm \sigma \sqrt{A}+\Delta p_{t}^{B R} \tag{20.2.1}
\end{equation*}
$$

where $p_{t}$ denotes the transverse momentum of the reconstructed jet, $p_{t, \text { hard }}$ the momentum of the original hard jet (in the absence of PU), $A$ the jet area, $\rho$ the background density per unit area within a given event, $\sigma$ the fluctuations of that background (per unit area) from place to place within the event, and $\Delta p_{t}^{B R}$ the back-reaction describing the effect of the background particles on the clustering of the hard ones.

If the background has a positional dependence (e.g. depends on rapidity) then $\rho$ and $\sigma$ will depend on the position of the jet one tries to subtract.

Eq. 20.2.1) characterises the fact that the background has the effects of shifting the transverse momentum of the jet and to degrade its resolution. The shift comes from the " $\rho$ " term in 20.2.1) and from potential back-reaction systematic effects. Using the anti- $k_{t}$ jet algorithm the shift due to backreaction is negligibl ${ }^{51}$. Resolution smearing effects come from various sources: the fluctuations of the background from within an event, i.e. the " $\sigma$ " term in 20.2.1, fluctuations of the background from one event to another, that is the fact that $\rho$ is not the same in every event, and the fluctuations in the back-reaction.

### 20.22 Central subtraction formula

From (20.2.1], the natural way to subtract the background contamination is to define the subtracted jet as [485]

$$
\begin{equation*}
p_{t, \text { sub }}=p_{t}-\rho_{\mathrm{est}} A \tag{20.2.2}
\end{equation*}
$$

where $\rho_{\text {est }}$ is the estimated value for the background density per unit area.
To apply this subtraction we need to compute the jet area and find an estimation $\rho_{\text {est }}$ for the background density per unit area. The jet areas are readily available using FastJet, so we just need to focus on $\rho_{\text {est }}$. The main goal of these proceedings is to investigate various methods of obtaining $\rho_{\text {est }}$ which are listed below. In all cases, it is primordial to realise that the determination of $\rho_{\text {est }}$ is performed event-by-event, and even jet-by-jet when the positional dependence of the background is taken into account.

As we shall see later on, the fact that $\rho$ is estimated for each individual event is crucial: it corrects for the fluctuations of the background from one event to another. If instead one uses an averaged value for $\rho_{\text {est }}$ (over many events), one would get an extra resolution smearing due to the fluctuations of $\rho$ across different events. Similarly, the jet area $A$ in 20.2.2) has to be computed for each individual jet. Using an average area would lead to an additional source of fluctuations of the form $\rho \sqrt{\left\langle A^{2}\right\rangle-\langle A\rangle^{2}}$.

[^235]Using seen vertices Since experimentally it might be possible - within some level of accuracy that goes beyond the scope of this discussion - to count the number of pileup vertices using charged track reconstruction, one appealing way to estimate the background density in a given event would be to count these vertices and subtract a pre-determined number for each of them:

$$
\begin{equation*}
\rho_{\mathrm{est}}^{(n \mathrm{PU})}(y)=f(y) n_{\mathrm{PU}, \text { seen }}, \tag{20.2.3}
\end{equation*}
$$

where we have made explicit the fact that the proportionality constant $f(y)$ can carry a rapidity dependence. $f(y)$ can be studied from minimum bias collisions (see Section 20.32 below) and can take into account the fact that only a fraction of the PU vertices will be reconstructed.

Median subtraction This technique divides the rapidity-azimuthal angle plane in patches and estimates $\rho$ for each event using

$$
\begin{equation*}
\rho_{\text {est }}^{(\text {global })}=\operatorname{median}_{i \in \text { patches }}\left\{\frac{p_{t, i}}{A_{i}}\right\} \tag{20.2.4}
\end{equation*}
$$

This is motivated by the observation that many regions in the event are populated just by the background. In these regions, $p_{t} / A$ is an estimate of $\rho$ and the use of the median, rather than the average, which ensures reduced bias from the hard jets.

This method was originally proposed in [485] using jets (from a $k_{t}$ or Cambridge/Aachen clustering) as patches. Here, we shall also test a new option where the $y-\phi$ plane is simply subdivided into grid cells that we use as patches.

Using a local range Eq. 20.2.4 provides a unique, global, estimate of $\rho$ for the event but does not take into account the positional-dependence of the background. One option, assuming one wants to estimate $\rho$ at the location of a jet $j$, is to limit the computation of the median to the jets in the vicinity of $j$, that i. 5

$$
\begin{equation*}
\rho_{\text {est }}^{(\text {local })}(j)=\underset{\text { jets } i \in \mathcal{R}(j)}{\operatorname{median}}\left\{\frac{p_{t, i}}{A_{i}}\right\} \tag{20.2.5}
\end{equation*}
$$

where $\mathcal{R}(j)$ is a local range around $j$. A typical example, that we shall study later on, is the case of a strip range where only the jets with $\left|y-y_{j}\right|<\Delta$ are included. This option was already proven to be powerful in [486].

Using rescaling Another option to correct for the rapidity dependence of the background ${ }^{53}$ is to introduce a pre-computed rapidity-reshaping function $f(y)$ (see Section 20.32) and use

$$
\begin{equation*}
\rho_{\text {est }}^{(\text {resc. })}(y)=f(y) \operatorname{median}_{i \in \text { patches }}\left\{\frac{p_{t, i}}{A_{i} f\left(y_{i}\right)}\right\} \tag{20.2.6}
\end{equation*}
$$

where now all patches (jets or grid cells) are included in the computation of the median.

### 20.3 Performance tests

### 20.31 Testing framework

The remainder of these proceedings will be devoted to an in-depth comparison of the subtraction methods proposed in Section 20.2. Our testing framework will be very similar to the one used in [486]: we embed a hard event into a pileup background (see again Section 20.2, we reconstruct and subtract the jets in

[^236]both the hard and full event $s^{54}$. for each jet in the hard event, we find the matching jet in the full event and compute the shift
\[

$$
\begin{equation*}
\Delta p_{t}=p_{t}^{\mathrm{full}, \mathrm{sub}}-p_{t}^{\mathrm{hard}, \mathrm{sub}}, \tag{20.3.1}
\end{equation*}
$$

\]

i.e. the difference between the reconstructed-and-subtracted jet with and without pileup. A positive (resp. negative) $\Delta p_{t}$ would mean that the PU contamination has been underestimated (resp. overestimated).

Though in principle there is some genuine information in the complete $\Delta p_{t}$ distribution - e.g. it could be useful to deconvolute the extra smearing brought by the pileup, see e.g. [486] and [487] - we shall focus on two simpler quantities: the average shift $\left\langle\Delta p_{t}\right\rangle$ and the dispersion $\sigma_{\Delta p_{t}}$. While the first one is a direct measure of how well one succeeds at subtracting the pileup contamination on average, the second quantifies the remaining effects on the resolution. One thus wishes to have $\left\langle\Delta p_{t}\right\rangle$ close to 0 and $\sigma_{\Delta p_{t}}$ as small as possible. Note that these two quantities can be studied as a function of variables like the rapidity and transverse momentum of the jets or the number of pileup interactions. In all cases, a flat behaviour would indicate a robust subtraction method.

The robustness of our conclusions can be checked by varying many ingredients:

- one can study various hard processes with the hope that the PU subtraction is not biased by the hard event. In what follows we shall study dijets with $p_{t}$ ranging from 50 GeV to 1 TeV , as well as fully hadronic $t \bar{t}$ events as a representative of busier final states.
- The Monte-Carlo used to generate the hard event and PU can be varied. For the hard event, we have used Pythia 6.4.24 [400] with the Perugia 2011 tune, Pythia 8.150 with tune 4C [348] and Herwig 6.5.10 [488] with the ATLAS tune and we have switched multiple interactions on (our default) or off. For the minimum bias sample used to generate PU, we have used Pythia 8, tune 4C, and checked that our conclusions remain unchanged when using Herwig++ [489] (tune LHC-UE7-2).

Additional details of the analysis For the sake of completeness, we list here the many other details of how the $\Delta p_{t}$ analysis has been conducted: we have considered particles with $|y| \leq 5$ with no $p_{t}$ cut or detector effect; jets have been reconstructed with the anti- $k_{t}$ algorithm with $R=0.5$ keeping jets with $|y| \leq 4$; for area computations, we have used active areas with explicit ghosts with ghosts placed ${ }^{55}$ up to $|y|=5$; for jet-based background estimations, we have used the $k_{t}$ algorithm with $R=0.4$ though other options will be discussed (and the 2 hardest jets in the set have been excluded from the median computation to reduce the bias from the hard event); for grid-based estimations the grid extends up to $|y|=5$ with cells of edge-size 0.56 (other sizes will be investigated); for estimations using a local range, a strip range of half-width 1.5 has been used and we refer to the Section 20.32 below for more information about the rapidity rescaling. Jet reconstruction, area computation and background estimation have all been carried out using FastJet (v3) [361, 435]. Pile-up is generated as a superposition of a Poissondistributed number of minimum bias events and we will vary the average number of pileup interactions. We shall always assume $p p$ collisions with $\sqrt{s}=7 \mathrm{TeV}$. Finally, the matching of a full jet to a hard jet is made by requiring that their common constituents contribute for at least $50 \%$ of the transverse momentum of the hard jet. We shall not discuss matching efficiencies here but they are extremely good: for a reconstructed (full) jet of 50 GeV and 20 PU events, the matching efficiency is $99.9 \%$ and this increases to $99.98 \%$ for $p_{t} \geq 50 \mathrm{GeV}$ and 5 PU events and $99.995 \%$ for $p_{t} \geq 100 \mathrm{GeV}$ and 20 PU events.

### 20.32 Minimum bias and rapidity shape

Before discussing the performances of the subtraction methods described in Section 20.2, there is still a building block that has to be discussed, namely the rapidity dependence of the background $f(y)$ that

[^237]

Fig. 105: Rapidity dependence of the transverse energy per unit area deposited in minimum bias events (obtained from Pythia 8, tune 4C). The normalisation of the fit is such that $f_{\text {seen }}$ is the fraction of seen minimum bias events i.e. the fraction of events which have at least 2 charged tracks with $|y| \leq 2.5$ and $p_{t} \geq 100 \mathrm{MeV}$.
enters in Eqs. 20.2.3) and 20.2.6). Letting aside the question of in-time vs. out-of-time PU and nonlinear effects in the detectors, the shape $f(y)$ can be obtained directly from minimum bias events.

In our case, we have generated minimum bias events with Pythia 8 (tune 4C) and studied the rapidity dependence of the transverse momentum deposited per unit area. The result is shown on Fig. 105 together with a quartic fit. If $f(y)$ is used to rescale median-based estimates of $\rho$, Eq. 20.2.6, any global normalisation factor would cancel, but in the case of Eq. 20.2.3) i.e. for the "seen vertices" method, the normalisation has to match what we mean by a seen PU vertex. In what follows, we shall define that as a minimum bias interaction that has at least 2 charged tracks with $|y| \leq 2.5$ and $p_{t} \geq 100$ MeV , which corresponds to $69.7 \%$ of the event ${ }^{56}$. In these conditions, we have found that the rapidity dependence is well reproduced by

$$
\begin{equation*}
f(y)=1.051141-0.023608 y^{2}+0.000026 y^{4} . \tag{20.3.2}
\end{equation*}
$$

### 20.33 Generic performance and rapidity dependence

Let us begin our performance benchmarks by the study of the rapidity dependence of PU subtraction. First of all, Fig. 106 shows the residual average shift $\left(\left\langle\Delta p_{t}\right\rangle\right)$ as a function of the rapidity of the hard jet. These results are presented for different hard processes, generated with Pythia 8 and assuming an average of 10 PU events per hard interaction. Robustness w.r.t. that choice will be discussed in the next Section but does not play any significant role for the moment.

The first observation is that the subtraction based on the number of seen PU vertices does a very good job in all 3 cases. Then, global median-based (using jets or grid cells) estimations of $\rho$, i.e. the (red) square symbols, do a fair job on average but, as expected, fail to correct for the rapidity dependence of the PU contamination. If one now restricts the median to a rapidity strip around the jet, the (blue) triangles, or if one uses rapidity rescaling, the (black) circles, the residual shift is very close to 0 , typically a few hundreds of MeV , and flat in rapidity.

Note that the strip-range approach seems to have a small residual rapidity dependence and overall offset for high- $p_{t}$ processes or multi-jet situations. That last point, more clearly observed with some

[^238]

Fig. 106: Residual average shift as a function of the jet rapidity for all the considered subtraction methods. For the left (resp. centre, right) plot, the hard event sample consists of dijets with $p_{t} \geq 50 \mathrm{GeV}$ (resp. dijets with $p_{t} \geq 400 \mathrm{GeV}$, and jets above $p_{t} \geq 50 \mathrm{GeV}$ in $t \bar{t}$ events), generated with Pythia 8 (tune 4 C ) in all cases. The typical PU contamination (for unsubtracted jets) is around 5 GeV .

Monte-Carlo generators like Pythia 6 than with others, may be due to the fact that smaller ranges tend to be more affected by the presence of the hard jets (see e.g. Appendix A. 2 of [486]), an effect which is reinforced for multi-jet events. The fact that the residual shift seems a bit smaller for grid-based estimates will be discussed more extensively in the next Section.

Next, we turn to the dispersion of $\Delta p_{t}$, a direct measure of the impact of PU fluctuations on the $p_{t}$ resolution of the jets. Our results are plotted in Fig. 107 as a function of the rapidity of the hard jet (left panel), the number of PU vertices (central panel) and the transverse momentum of the hard jet (right panel). All subtraction methods have been included as well as the dispersion one would observe if no subtraction were performed.

The results show a clear trend: first, a subtraction based on the number of seen PU vertices bring an improvement compared to not doing any subtraction; second, median-based estimations of $\rho$ give a more significant improvement; and third, all median-based approaches perform similarly well.

The reason why median-based estimations of $\rho$ outperform the estimation based on the number of seen PU vertices is simply because minimum bias events do not all yield the same energy deposit and this leads to an additional source of fluctuations in the "seen vertices" estimation compared to all median-based ones. This is the main motivation for using an event-by-event determination of $\rho$ based on the energy deposited in the event. This motivation is further strengthened by the fact that additional issues like vertex resolution or out-of-time PU would affect both $\left\langle\Delta p_{t}\right\rangle$ and $\sigma_{\Delta p_{t}}$ if estimated simply from the number of seen vertices while median-based approaches are more robust.

Note finally that even though local ranges and rapidity rescaling do correct for the rapidity dependence of the PU on average, the dispersion still depends on rapidity. The increase with the number of PU vertices is in agreement with the expected $\sqrt{n_{\mathrm{PU}}}$ behaviour and the increase with the $p_{t}$ of the hard process can be associated with back-reaction, see [486]. These numbers can also be compared to the typical detector resolutions which would be $\sim 10 \mathrm{GeV}$ for 100 GeV jets and $\sim 20 \mathrm{GeV}$ at $p_{t}=400 \mathrm{GeV}$ [490, 491].

### 20.34 Robustness and Monte-Carlo dependence

The last series of results we want to present addresses the stability and robustness of the median-based estimation of the PU density per unit area.

To do that, the first thing we shall discuss is the Monte-Carlo dependence of our results. In Fig.


Fig. 107: Dispersion $\sigma_{\Delta p_{t}}$. Each curve corresponds to a different subtraction method and the results are presented as a function of different kinematic variables: left, as a function of the rapidity of the hard jet for a sample of jets with $p_{t} \geq 100 \mathrm{GeV}$ and assuming an average of 10 PU events; centre: as a function of the number of PU events for a sample of jets with $p_{t} \geq 100$; right: as a function of the $p_{t}$ of the hard jet, assuming an average of 10 PU events


Fig. 108: Dependence of the average $p_{t}$ shift as a function of the number of PU vertices for various Monte-Carlo generators. For the left plot, the hard sample is made of dijets with $p_{t} \geq 100 \mathrm{GeV}$ while for the right plot, we have used a hadronic $t \bar{t}$ sample. For each generator, we have considered both the case with the Underlying Event switched on (filled symbols) and off (open symbols). All results have been obtained using a grid-based median estimation of $\rho$ using rapidity rescaling.


Fig. 109: Average residual shift after PU subtraction. $\left\langle\Delta p_{t}\right\rangle$ is plotted as a function of the $p_{t}$ of the jet for an average of 10 PU events (left panel), or as a function of the number of PU vertices for dijets with $p_{t} \geq 100 \mathrm{GeV}$ (central panel) and for $t \bar{t}$ events (right panel). In all cases, we compare 3 methods: the rapidity-strip range, (red) triangles, the jet-based approach with $y$-rescaling, (blue) circles, and the gridbased approach with $y$ rescaling, (black) squares. Each curve is the result of averaging over the various Monte-Carlo generator options and the dispersion between them is represented both as error bars on the top row and directly on the bottom row.

108 we compare the different Monte-Carlo predictions for the $\left\langle\Delta p_{t}\right\rangle$ dependence on the number of PU vertices in the case of a grid-based median estimate of $\rho$ with rapidity rescaling. For each of the three considered Monte-Carlos, we have repeated the analysis with and without Underlying Event (UE) in the hard event. The first observation is that all the results span a range of $300-400 \mathrm{MeV}$ in $\Delta p_{t}$ and have a similar dependence on the number of PU vertices. The dependence on $n_{\mathrm{PU}}$ is flat for dijet events but shows a small decrease for the busier $t \bar{t}$ events. The $300-400 \mathrm{MeV}$ shift splits into a $100-200 \mathrm{MeV}$ effect when changing the generator, which is likely due to the small but non-zero effect of the hard event on the median computation, and a $100-200 \mathrm{MeV}$ effect coming from the switching on/off of the UE.

This question of subtracting the UE deserves a discussion: since the UE is also a soft background which is relatively uniform, it contributes to the median estimate and, therefore, one expects the UE, or at least a part of it, to be subtracted together with the PU. Precisely for that reason, when we compute $\Delta p_{t}$, our subtraction procedure is not applied only on the "full jet" (hard jet+PU) but also on the hard jet, see Eq. 20.3.1. The $100-200 \mathrm{MeV}$ negative shift observed in Fig. 108 thus means that, when switching on the UE, one subtracts a bit more of the UE in the full event (with PU) than in the hard event alone (without PU). This could be due to the fact (see [492] for details) that for sparse events, as is typically the case with UE but no PU, the median tends to slightly underestimate the "real" $\rho$, e.g. if half of the event is empty, the median estimate would be 0 . This is in agreement with the fact that for $t \bar{t}$ events, where the hard event is busier, switching on the UE tends to have a smaller effect. Note finally that as far as the size of the effect is concerned, this $100-200 \mathrm{GeV}$ shift has to be compared with the $\sim 1 \mathrm{GeV}$ contamination of the UE in the hard jets.

Finally, we wish to compare the robustness of our various subtraction methods for various processes i.e. hard events and PU conditions. In order to avoid multiplying the number of plots, we shall treat the Monte-Carlo (including the switching on/off of the UE) as an error estimate. That is, an average measure and an uncertainty will be extracted by taking the average and dispersion of the 6 Monte-Carlo setups. The results of this combination are presented on Fig. 109 for various situations and subtraction


Fig. 110: Left: relative difference between the reconstructed jet and the reconstructed $Z$ boson transverse momenta. Right: at a given $p_{t}$ of the reconstructed $Z$ boson, difference between the reconstructed $p_{t}$ of the jet and the ideal $p_{t}$ with no UE or PU, i.e. $p_{t}$ shift w.r.t. the "noUE" curve, the (black) triangles, on the left panel. See the text for the details of the analysis.
methods. For example, the 6 curves from the left plot of Fig. 108 have been combined into the (black) squares of the central panel in Fig. 109 .

Two pieces of information can be extracted from these results. First of all, for dijets, the quality of PU subtraction is, to a large extent, flat as a function of the $p_{t}$ of the jets and the number of PU vertices. When moving to multi-jet situations, we observe an additional residual shift in the $100-300 \mathrm{MeV}$ range, extending to $\sim 500 \mathrm{MeV}$ for the rapidity-strip-range method. This slightly increased sensitivity of the rapidity-strip-range method also depends on the Monte-Carlo. While in all other cases, our estimates vary by $\sim 100 \mathrm{MeV}$ when changing the details of the generator, for multi-jet events and the rapidity-strip-range approach this is increased to $\sim 200 \mathrm{MeV}$.

Overall, the quality of the subtraction is globally very good. Methods involving rapidity rescaling tends to perform a bit better than the estimate using a rapidity strip range, mainly a consequence of the latter's greater sensitivity to multi-jet events. In comparing grid-based to jet-based estimations of $\rho$, one sees that the former gives slightly better results, though the differences remain small.

Since the grid-based approach is considerably faster than the jet-based one, as it does not require an additional clustering of the even ${ }^{57}$, the estimation of $\rho$ using a grid-based median with rapidity rescaling comes out as a very good default for PU subtraction. One should however keep in mind local-range approaches for the case where the rapidity rescaling function cannot easily be obtained.

### 20.4 PU v. UE subtraction: an analysis on $Z+j e t$ events

To give further insight on the question of what fraction of the Underlying Event gets subtracted together with the pileup, we have performed an additional study of $Z+$ jet events. We look at events where the $Z$ boson decays into a pair of muons. We have considered 5 different situations: events without PU or UE, events with UE but no PU subtracted or not, and events with both UE and PU again subtracted or not. Except for the study of events without UE, this analysis could also be carried out directly on data.

Practically, we impose that both muons have a transverse momentum of at least 20 GeV and have $|y| \leq 2.5$, and we require that their reconstructed invariant mass is within 10 GeV of the nominal $Z$

[^239]mass. As previously, jets are reconstructed using the anti- $k_{t}$ jet algorithm and the pileup subtraction is performed using the grid-based-median approach with rapidity rescaling and a grid size of 0.55 . All events have been generated with Pythia 8 (tune 4C) and we have assumed an average PU multiplicity of 20 events.

In Fig. 110, we have plotted the ratio $p_{t, \text { jet }} / p_{t, Z}-1$, with $p_{t, \text { jet }}$ the transverse momentum of the leading jet, for the various situations under considerations. Compared to the ideal situation with no PU and no UE, the (black) triangles, one clearly sees the expected effect of switching on the UE, the empty (green) circles, or adding PU, the empty (red) squares: the UE and PU add to the jet $\sim 1.2$ and 13 GeV respectively.

We now turn to the cases where the soft background is subtracted, i.e. the filled (blue) squares and (magenta) circles, for the cases with and without PU respectively. There are two main observations:

- with or without PU, the UE is never fully subtracted: from the original $1-1.5 \mathrm{GeV}$ shift, we do subtract about 800 MeV to be left with a $0-500 \mathrm{MeV}$ effect from the UE. That effect becomes smaller and smaller when going to large $p_{t}$.
- in the presence of PU, the subtraction produces results very close to the corresponding results without PU and where only the UE is subtracted. This nearly perfect agreement at large $p_{t, \text { jet }}$ slightly degrades into an additional offset of a few hundreds of MeV when going to smaller scales. This comes about for the following reason: the non-zero $p_{t}$ resolution induced by pileup (even after subtraction) means that in events in which the two hardest jets have similar $p_{t}$, the one that is hardest in the event with pileup may not correspond to the one that is hardest in the event without pileup. This introduces a positive bias on the hardest jet $p_{t}$ (a similar bias would be present in real data even without pileup, simply due to detector resolution). The "matched" curve in Fig. 110 (right) shows that if, in a given hard event supplemented with pileup, we explicitly use the jet that is closest to the hardest jet in that same event without pileup, then the offset disappears, confirming its origin as due to resolution-related jet mismatching.


### 20.5 Conclusions and discussion

In these proceedings, we have investigated several methods to correct for the pile-up contamination to jets. They are all based on the observation that the average PU contribution to a jet is on average proportional to its area, which directly leads to eq. 20.2.2. The various methods then differ by the method used to estimate the PU activity per unit area, $\rho$. The subtraction efficiency has been studied by embedding hard events into PU backgrounds and investigating how jet reconstruction was affected by measuring the remaining $p_{t}$ shift after subtraction $\left(\left\langle\Delta p_{t}\right\rangle\right)$ as well as the impact on resolution ( $\sigma_{\Delta p_{t}}$ ).

There are 3 broad approaches to the estimation of $\rho$ : (a) using an average contamination per PU vertex, the seen vertices approach, (b) using an event-by-event estimation and, the median approach with jets or grid cells as patches, and (c) using an event-by-event and jet-by-jet method, the local range or rescaling approaches.

The first important message is that, though all methods give a very good overall subtraction $\left(\left\langle\Delta p_{t}\right\rangle \approx 0\right.$ ), event-by-event methods should be preferred because their smaller PU impact on the $p_{t}$ resolution (see Fig. 107). This is mostly because the "seen vertices" method has an additional smearing coming from the fluctuations between different minimum bias collisions. This does not happen in event-by event methods that are only affected by point-to-point fluctuations in an event. Note also that event-by-event methods are very likely more robust than methods based on identifying secondary vertices when effects like vertex identification and out-of-time PU are taken into account.

The next observation is that event-by-event and jet-by-jet methods have the additional advantage that they correct for positional-dependence of the background like its rapidity dependence (see Fig. 106). The median approach using a local range (with jets as patches) or rapidity rescaling (using jets or grid cells as patches) all give an average offset in the $0-300 \mathrm{MeV}$ range, independently of the rapidity of
the jet, its $p_{t}$ or the number of PU vertices, see Fig. 109 and are thus very suitable methods for PU subtraction at the LHC. Pushing the analysis a bit further one may argue that the local-range method has a slightly larger offset when applied to situations with large jet multiplicity like $t \bar{t}$ events (the right panel of Fig. (109) though this argument seems to depend on the Monte-Carlo used to generate the hard-event sample. Also, since it avoids clustering the event a second time, the grid-based method has the advantage of being faster than the jet-based approach.

At the end of the day, we can recommend the median-based subtraction method with rapidity rescaling and using grid cells as patches as a powerful default PU subtraction method at the LHC. But one should keep in mind that the use of jets instead of grid cells also does a very good job and that local-ranges can be a good alternative to rapidity rescaling if the rescaling function cannot be computed. Also, though we have not discussed that in detail, a grid cell size of 0.55 is a good default as is the use of $k_{t}$ jets with $R=0.4$.

To conclude, let us make a few general remarks. First, our suggested method involves relatively few assumptions, which helps ensure its robustness. Effects like in-time v. out-of-time PU or detector response should not have a big impact. Many of the studies performed here can be repeated with "real data" rather than Monte-Carlo simulations. The best example is certainly the $Z+$ jet study of Section 20.4 which could be done using data samples with different PU activity from 2010 and 2011. Also, the rapidity rescaling function can likely be obtained from minimum bias collision data and the embedding of a hard event into pure PU events could help quantifying the remaining $\mathcal{O}(100 \mathrm{MeV})$ bias. Experimentally, it would also be interesting to investigate hybrid techniques where one would discard the charged tracks that do not point to the primary vertex and apply the subtraction technique described here to the rest of the event. This would have the advantage to further reduce fluctuation effects (roughly by a factor $\sim \sqrt{1 /\left(1-f_{\mathrm{chg}}\right)} \approx 1.6$, where $f_{\mathrm{chg}} \approx 0.61$ is the fraction of charged particles in an event). Finally, all the facilities to compute jet areas and background estimation - including jets or grid-cells as patches, local ranges and rescaling functions - are readily available from FastJet (v3.0.0 onward) using e.g. the GridMedianBackgroundEstimator or Subtractor tools.

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## Part VI

## MC TUNING AND OUTPUT FORMATS

## 21. TUNE KILLING: QUANTITATIVE COMPARISONS OF MC GENERATORS AND TUNES ${ }^{58}$


#### Abstract

We summarise the implementation, status, and scope of the "tune killing" project, which classifies MC generator codes and tunes according to their quality of data description across a range of LHC-relevant observables. The primary aim of the project is to provide sufficiently clear information about generator performance that the current large collection of available tunes may be objectively reduced to a more manageable standard set for common use by LHC experiments and phenomenologists. We make final recommendations as


[^240]to which generators and tunes are in rude health, and those which are obvious candidates for retirement from active service.

### 21.1 INTRODUCTION

Popular MC generators are nowadays associated with a bewildering array of standard parameter configurations, called "tunes". This proliferation of tunes is due to the ongoing project to provide optimised descriptions of LEP, Tevatron and LHC data: as new data and techniques have become available, new tunes have been created, usually but not always with increasing quality of data description. This process looks set to continue, and hence there is a need for agreement on which tunes are of most common interest at a given time.
The PYTHIA6 [400] event generator in particular has been the de facto testbed for tuning due to the wealth of community expertise and its ubiquity of tuning parameters for physical processes. At the time of writing there are 77 tunes available via the built-in PYTUNE routine, and a further 10 or more presented by the ATLAS experiment alone (this counting of ATLAS tunes includes equivalently weighted tunes for multiple PDFs, but not systematic variation tunes, of which there are many more). With such a profligacy of configuration options, it is difficult to objectively decide which are to be preferred for LHC simulation without manually cross-referencing hundreds of plots. It is hence not uncommon for different experimental or phenomenological studies to use entirely disjoint MC generator setups, making comparison difficult. Ideally we would have a much smaller set of agreed-upon generator setups, but choosing such a privileged subset requires clear information on which to base our preferences.
As a first step to addressing this issue, we present here a comparative study of event generator codes and tunes across a range of observables, particularly those of relevance for LHC physics. The study is based on analyses from the Rivet [360] toolkit, and the resulting data descriptions are quantitatively scored based on measures of deviation from the data values, including $\chi^{2}$ and median/maximum binwise deviations (in units of combined experimental, statistical, and theoretical uncertainties). The results are presented as a series of Web pages, using colour coded tables which are hyperlinked to provide the necessary information in a compact, hierarchical form.

### 21.2 Analysis system

The data analysed for this project was produced by individual runs of various generator/tune configurations into the Rivet analysis system. A choice of Rivet analyses was made, intended to cover a number of core QCD modelling aspects for LHC physics: these are documented in Table 16. In some cases only the most relevant range in the distribution is included, as indicated in the Table. The generators and tunes used are documented in Table 17
Note that not all observables are suitable for all generators. For example, AlpGen has not been used for LEP fragmentation, although in a future iteration we will extend the AlpGen coverage to include underlying event observables, where the hard jets could interfere with those from the multiple parton interaction (MPI) mechanism. Several observables, notably hard photon physics, minimum bias observables, and fragmentation/strangeness from RHIC and LHC have not yet been included: this is envisaged as a future extension of the project.
A Python program was written to load the histogram files for each generator/tune combination from a hierarchical directory structure, and to perform some basic statistical characterisation on each bin, histogram, and semantic group of histograms. At the histogram level, specifications are used to determine which bins are to be considered in the statistical comparisons, and to add a nominal "theoretical uncertainty". In this study a $10 \%$ theoretical uncertainty was added to the underlying event and fragmentation observables and a $5 \%$ theoretical uncertainty on the rest. The combined uncertainty for each bin $b$ is then computed from the sum in quadrature of the reference data error, the MC statistical error and the theoretical uncertainty, and is used to compute a MC-data deviation for that bin, expressed in units of

| Observable | Rivet analysis | Ref. | Range |
| :---: | :---: | :---: | :---: |
| Underlying event |  |  |  |
| Transverse region $N_{\text {ch }}$ vs. $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Transverse region $\sum p_{\perp}$ vs. $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Transverse region $\left\langle p_{\perp}\right\rangle$ vs $N_{\text {ch }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] |  |
| Jets |  |  |  |
| Toward region $N_{\text {ch }}$ vs $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Toward region $\sum p_{\perp}$ vs $p_{\perp}^{\text {lead }}, p_{\perp}^{\text {ch }}>500 \mathrm{MeV}$ | ATLAS_2010_S8894728 | [493] | $p_{\perp}^{\text {lead }}>5 \mathrm{GeV}$ |
| Jet shapes, $30<p_{\perp}<40 \mathrm{GeV}$, $\|y\|<2.8$ | ATLAS_2011_S8924791 | [494] |  |
| Jet shapes, $310<p_{\perp}<400 \mathrm{GeV},\|y\|<2.8$ | ATLAS_2011_S8924791 | [494] |  |
| Dijet $\Delta \phi, 110<p_{\perp}<160 \mathrm{GeV}$ | ATLAS_2011_S8971293 | [495] | $3 \pi / 4 \rightarrow \pi$ |
| Dijet $\Delta \phi, 310<p_{\perp}<400 \mathrm{GeV}$ | ATLAS_2011_S8971293 | [495] | $3 \pi / 4 \rightarrow \pi$ |
| Dijet mass, $0.3<\|y\|<0.8$, anti- $k_{\perp}(0.4)$ | ATLAS_2010_S8817804 | [382] |  |
| Transverse thrust, $90 \mathrm{GeV}<p_{\perp}^{\text {jet1 }}<125 \mathrm{GeV}$ | CMS_2011_S8957746 | [496] |  |
| ISR/intrinsic- $k_{\perp}$ |  |  |  |
| DØ $\phi^{*},\|y\|<1.0$ | D0_2010_S8821313 | [497] | $\phi^{*}<0.4$ |
| DØ $\phi^{*}, 1.0<\|y\|<2.0$ | D0_2010_S8821313 | [497] | $\phi^{*}<0.4$ |
| Fragmentation |  |  |  |
| $N_{\text {ch }}, \pi^{+} / \pi^{-}, K^{+} / K^{-}$at LEP | DELPHI_1996_S3430090 | [498] |  |
| $\rho / \pi, K / \pi, \Sigma^{ \pm,+,-, 0} / \pi, p / \pi, \Lambda / \pi$ | PDG_HADRON_MULTIPLICITIES | [499] |  |
| Inclusive $x_{p}$, thrust (+ major \& minor) | DELPHI_1996_S3430090 | [498] |  |
| $B$ fragmentation | DELPHI_2002_069_CONF_603 | [500] |  |

Table 16: Observables used in the tune killing exercise.

| Generator and version | Tunes |
| :--- | :--- |
| Sherpa 1.3.1[[146] | Default (CTEQ6.6) |
| Herwig++ 2.5.2[489] | LHC-UE-EE-3 series (LO $* *$ and CTEQ6L1) |
| Pythia 8.150[348] | 4C |
| PYTHIA 6.425[400] | D6T, DW[501], Z2, AMBT1[502], AUET2B (LO $* *$ and CTEQ6L1)[503], |
|  | Perugia 2010[504], Perugia 2011[504], prof- Q $^{2}[451]$ |
| AlpGen[505] + PYTHIA 6.425 $\left(^{*}\right)$ | Same tunes as PYTHIA6. |
|  | Perugia 2011 using matched ME/PS $\Lambda_{\mathrm{QCD}} \cdot[506]$ |
| HERWIG 6.510[488] + JIMMY 4.31[507] | AUET2 LO $* *[508]$ |
| AlpGen + HERWIG 6.5 + JIMMY 4.31 $\left(^{*}\right)$ | Same as for HERWIG+JIMMY. |

Table 17: Generators and tunes used in the tune killing exercise. (*) Jet and $Z$ boson $\phi^{*}$ observables only.
the total bin error, $\operatorname{dev}_{b}=\left(\mathrm{MC}_{b}-\operatorname{data}_{b}\right) / \operatorname{err}_{b}$.
For each active histogram, the system then reports the $\chi^{2} / N_{\text {bin }}$, and the median, mean, and maximum bin-wise deviation. A total "metric" value for each histogram is reported as the maximum bin-wise deviation if that is greater than $10 \sigma$, otherwise the greater of the median and mean deviations. This hybrid treatment of the metric allows the system to flag up histograms in which there are either widespread moderate deviations or a small number of very discrepant bins which might be missed with a pure median or mean deviation treatment. An HTML table and set of histograms are rendered by the system for each observable, with a continuous colour coding scheme used to highlight the relative quality of data description from ideal (green) to very poor (red).
The histograms are grouped to collect together observables from different sources which reflect related aspects of QCD modelling. The current groups are "Underlying Event (UE)", "Dijets", "Multijets", "Jet shapes", "W and Z", "Fragmentation", and " $B$ fragmentation". In these groups, the same $\chi^{2} / N_{\text {bin }}$, and mean/median/maximum deviation statistics are calculated as before. For visual compactness of classification we again use a hybrid performance metric for each histogram group: again this is the maximum bin-wise deviation found in the contained histograms if that is greater than $10 \sigma$, otherwise the maximum histogram-wise deviation metric in the group if that is greater than $5 \sigma$, otherwise the maximum of the median/mean bin-wise deviation.
The Web pages generated to present this data in a compact way consist of a single top level page containing a colour-coded table of tune performance metrics for each histogram group. Each cell in the table is hyperlinked to a more detailed table for that tune/group where the various $\chi^{2} / N$, max/mean/median deviation and hybrid metric are presented, again colour-coded, for each histogram in the group. The table rows are then hyperlinked to a plot page showing explicitly the tune/generator behaviour for each histogram and indicating the active range of the histograms where appropriate. These pages are shown in Figures 111 to 113 . This form of presentation allows a rapid assessment of generator/tune performance, while still permitting detailed investigation of any flagged-up issues with a few mouse clicks. The system is easily extensible to more observables, groups, and different theory uncertainty / visual classification thresholds.
The classification colours for each performance figure are generated in HSB colour space as a linear variation in deviation $x$ between green (120) and red (0) in the Hue parameter, i.e. $H=120(1-$ $\left.\min \left(x / x_{\text {bad }}, 1.0\right)\right)$, with fixed Saturation and Brightness parameters. The visual threshold $x_{\text {bad }}$ was chosen to be different for each metric type: $5 \sigma$ for maximum deviations, $4 \sigma$ for $\chi^{2} / N$, and $2 \sigma$ for mean and median deviations, and for the hybrid performance metrics. These thresholds were iterated from initial suggestions to the point where distinctions could be made between the models: similar iteration of the discriminating criteria are envisaged while significant model/tune variations exist as the motivation of this study is model discrimination rather than passing or failing a natural performance figure.

### 21.3 Results

As the central theme of this project has been to provide a comprehensible visualisation of the relative performance of generators and tunes, and hierarchical presentation via Web pages was key to achieving this, it would be self-defeating to attempt to present the same information in this summary. Additionally, the nature of tune comparison is that it evolves as new data, tunes, and generator versions become available. Hence, for up-to-date status information we refer the reader to the persistent "tune killing" web page at http:/ /projects.hepforge.org/rivet/tunecmp/.
However, it is worth mentioning some of the most striking features of generators which have been made more evident by this collating of data-MC comparisons:

- The general quality of jet and W/Z data description is in fact better than expected: among PYTHIA tunes in particular there is sufficient variation in parton shower parameters that significant deviations in jet observables would reasonably be expected, but in fact the majority of tunes describe


## Tune comparisons

Deviation metrics per gen/tune and observable group:

| Gen | Tune | UE | Dijets | Multijets | Jet shapes | W and Z | Fragmentation | B frag |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AlpGen | HERWIG6 | - | 1.83 | 5.36 | 2.48 | 0.91 | - | - |
|  | PYTHIA6-AMBT1 | - | 1.55 | 2.80 | 0.61 | 0.53 | - | - |
|  | PYTHIA6-D6T | - | 1.38 | 2.67 | 2.31 | 1.67 | - | - |
|  | PYTHIA6-P2010 | - | 1.09 | 2.65 | 2.03 | 1.48 | - | - |
|  | PYTHIA6-P2011 | - | 1.12 | 2.60 | 0.48 | 0.24 | - | - |
|  | PYTHIA6-Z2 | - | 1.48 | 2.63 | 0.55 | 0.48 | - | - |
|  | PYTHIA6-profQ2 | - | 1.16 | 2.65 | 1.43 | 1.29 | - | - |
| HERWIG | AUET2-CTEQ6L1 | 0.43 | 0.55 | 0.77 | 0.35 | 0.58 | 22.80 | 2.38 |
|  | AUET2-LOxx | 0.25 | 0.71 | 0.60 | 0.39 | 0.88 | 22.13 | 2.29 |
| Herwig++ | 2.5.1-UE-EE-3-CTEQ6L1 | 0.27 | 0.87 | 0.78 | 0.51 | 0.98 | 10.58 | 1.32 |
|  | 2.5.1-UE-EE-3-MRSTLOxx | 0.23 | 1.05 | 0.78 | 0.50 | 0.65 | 10.58 | 1.32 |
| PYTHIA6 | AMBT1 | 0.39 | 1.20 | 0.54 | 0.77 | 0.27 | 0.93 | 1.65 |
|  | AUET2B-CTEQ6L1 | 0.16 | 0.92 | 0.44 | 0.59 | 0.74 | 0.67 | 1.29 |
|  | AUET2B-LOxx | 0.13 | 1.33 | 0.55 | 0.58 | 1.15 | 0.67 | 1.30 |
|  | D6T | 0.58 | 0.79 | 0.50 | 0.56 | 1.25 | 0.36 | 2.63 |
|  | DW | 0.81 | 0.78 | 0.61 | 0.56 | 1.33 | 0.36 | 2.63 |
|  | P2010 | 0.30 | 0.93 | 0.82 | 1.07 | 0.30 | 0.44 | 1.75 |
|  | P2011 | 0.12 | 0.89 | 0.67 | 1.02 | 0.53 | 0.43 | 2.13 |
|  | ProfQ2 | 0.51 | 0.67 | 0.81 | 0.51 | 0.64 | 0.30 | 1.65 |
|  | Z2 | 0.18 | 0.94 | 0.73 | 0.80 | 0.30 | 0.95 | 2.78 |
| Pythias | 4 C | 0.30 | 0.97 | 0.93 | 0.50 | 0.90 | 0.38 | 1.12 |
| Sherpa | 1.3.1 | 0.68 | 0.47 | 0.34 | 0.71 | 0.36 | 0.75 | 2.48 |

Fig. 111: Screenshot of the top-level summary page produced by the tune comparison system.
Jet shapes

| Histo | chi2/Nat | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Jet shape svinos for Sp_\.... (ATLAS_2011_S8924791/d01-x06-y01) | 0.59 | 0.77 | 0.69 | 1.17 | 0.77 |
| jet shape Svihos for Sp_lp... (ATLAS_2011_58924791/d09-×06-y01) | 0.14 | 0.36 | 0.30 | 0.61 | 0.36 |
| Central Transv. Thrust, $59 \ldots$ (CMS_2011_ $58957746 / 101 \times \times 01$-y01) | 0.37 | 0.43 | 0.53 | 1.08 | 0.53 |
| Central Transv. Minor, 590... (CMS_2011_58957746/d02-x01-y01) | 0.34 | 0.38 | 0.48 | 1.14 | 0.48 |

## W and Z

| Histo | chi2/Ndf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Muon channel ( $\mathrm{s} \mid \mathrm{y}$ _ $\mathrm{Z} \mid<1 \mathrm{~s}$ ) (D0_2010_ $58821313 / 802$-x01-y01) | 0.77 | 0.70 | 0.79 | 1.52 | 0.79 |
| Muon channel ( $\$ 1<\mid y \mathrm{z}$ Z\|<2s) (00_2010_s8821313/d02-x01-y02) | 0.27 | 0.38 | 0.45 | 1.08 | 0.45 |

## Fragmentation

| Histo | chi2/Wdf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Scaled momentum, 5x.p = \|p... (DELPH1_1996_S3430090/d07-x01-y01) | 0.74 | 0.28 | 0.47 | 3.29 | 0.47 |
| S1-text(Thrust)s (DELPHI_1996_S3430090/d11-x01-y01) | 4.12 | 0.24 | 1.13 | 8.26 | 1.13 |
| Thrust major, SMS (DELPH1_1996_53430090/d12-x01-y01) | 7.24 | 0.50 | 1.61 | 9.37 | 1.61 |
| Thrust minor, sms (DELPH1_1996_53430090/d13-x01-y01) | 9.69 | 0.40 | 1.57 | 10.58 | 10.58 |
| Mean charged mutitilicity (DELPH1_1996_S3430090/d35-x01-y01) | 0.08 | 0.28 | 0.28 | 0.28 | 0.28 |

Fig. 112: Screenshot of the mid-level performance metric page produced by the tune comparison system. This specific example is part of the performance metrics for the Herwig++ LHC-UE-EE-3 LO $* *$ tune.

## Plots for PYTHIA6, AUET2B-LOxx, B frag



Fig. 113: Screenshot of the observable plot page produced by the tune comparison system. This specific example shows the $B$ fragmentation performance of the PYTHIA6 AUET2B LO** tune.
data fairly well.

- The UE in particular has been a focus of tuning activity and this is evident in the consistency of UE data description. The worst performance in this group is from the DW tune of PYTHIA, but even this pre-LHC tune with the "old" PYTHIA MPI model achieves a deviation metric of less than $1 \sigma$ on LHC UE observables.
- PYTHIA D6T outperforms PYTHIA DW - an unexpected result since the MPI energy evolution of D6T is fixed to the default and disfavoured form $p_{\perp}^{0}(s) \sim(\sqrt{s} / 1800 \mathrm{GeV})^{0.16}$, whereas the exponent in DW is closer to the tuned consensus of $\sim 0.25$. This may be a lucky behaviour at 7 TeV , and hence care is needed with extrapolation of D6T to 8,10 , or 14 TeV , but it is clear that the PYTHIA $Q^{2}$-ordered parton shower is not yet dead on purely physics grounds. The best tune of this PYTHIA configuration, however, is Prof- $Q^{2}$, which in addition to general small improvements, is significantly better than DW or D6T at describing the vector boson $p_{\perp}$ distribution.
- Pythia8 is generally seen to perform very well, and provides significant improvements over PYTHIA6 for jet shapes and $B$ fragmentation. Tuning focus is accordingly beginning to shift towards Pythia8, also for minimum bias observables not yet considered here.
- AlpGen interacts strongly with tunes on jet shape and vector boson data descriptions. In particular there appears to be little motivation to use AlpGen with the D6T or Perugia 2010 tunes of PYTHIA6. AlpGen+HERWIG also has significant problems with jet shapes in particular, and the indication of this study is that AlpGen+PYTHIA Perugia 2011 is the most performant configuration, closely followed by AlpGen+PYTHIA Z2. Notably, the Perugia 2011 tune of PYTHIA was specifically developed to minimise ME/PS merging artefacts when used with AlpGen.
- Both HERWIG and Herwig++ have problems describing LEP fragmentation data, but Herwig++ is a very significant improvement over its Fortran cousin. The identified hadron rates are in particular much improved, although $K^{ \pm}$and $\Sigma^{0}$ remain anomalous. However, a known problem with Herwig++ is the poor description of the LEP thrust distribution, which overshoots significantly in the multi-parton region.
- AlpGen seems to have difficulty describing dijet azimuthal decorrelations, even when restricted to the $2 / 3$ parton region of the plot. This is particularly surprising as AlpGen is intended to provide
the multi-parton configurations needed to describe this observable.
- $B$ fragmentation is in general quite poorly described. The best descriptions are by Pythia8, the AUET2B tunes of PYTHIA6, and Herwig++. Other generators and tunes are in decidedly dodgy shape for $B$-specific predictions at the LHC.
Insofar as it is within the scope of this project to make recommendations for canonical generator and tune choices, we note that the Perugia 2011, AUET2B, and Z 2 tunes of PYTHIA6 provide the best data descriptions currently available with that generator and that the Prof- $Q^{2}$ tune is the best available configuration using the $Q^{2}$-ordered PYTHIA parton shower. We hence recommend these 4 PYTHIA tunes as the current minimal set of PYTHIA tunes for general use at the LHC, particularly once an update of the ATLAS AUET2B tune has fixed the tuning issue with the $Z p_{\perp}$.
Among the other generators, where there is not such a proliferation of tunes, we note again the apparent performance issues with AlpGen - this is clearly in need of further pursuit. However, to reduce the amount of comparison needed, we note that Perugia 2011 is the only PYTHIA6 tune now optimised for use with AlpGen with avoidance of the worst effects of ME/PS coupling mismatches: hence future studies can quite happily restrict themselves to this AlpGen+PYTHIA configuration. As AlpGen+HERWIG has several problems with jet description, HERWIG itself has serious problems with both light and $B$ fragmentation, and no further tuning of the JIMMY MPI model is envisaged, the HERWIG generator cannot be recommended for future use in any capacity where an alternative exists.
The "new" C++ generators Herwig++, Pythia8, and Sherpa all perform well, with the exception of Sherpa's $B$ fragmentation and the Herwig++ light fragmentation. Pythia8 generally behaves well but some tuning or development may be needed to improve inter-jet observables and the $Z p_{\perp}$ spectrum. In general, the $\mathrm{C}++$ generators are in good health, and we anticipate further improvements as the focus of tuning studies shifts to them.


### 21.4 Outlook

This project has put in place a system and a set of classification criteria which have proven useful for summarising and investigating MC generator model and tune predictivity for a variety of QCD phenomena. While we claim no mandate to truly "kill" certain tunes or generators, and wish to emphasise that a poor performance in a single observable type (in particular $B$ fragmentation) certainly does not render that generator useless, the results from these comparisons do provide strong arguments for deprecation of at least several PYTHIA6 tunes and of the Fortran HERWIG generator in general.
It is the nature of a project like this that results are continually being updated, and there are many natural avenues for extension which we wish to pursue, in particular:

- Extra observables, e.g. minimum bias and $E_{\perp}$ flow, LHC and Tevatron photon physics, LHC $W / Z$ $p_{\perp}$ data, strangeness data from LHC and RHIC, explicit multijet observables, etc..
- Extra generators and tunes, in particular POWHEG+PYTHIA/HERWIG/Pythia8/Herwig++, MadGraph+PYTHIA/Pythia8, MC@NLO+HERWIG/Herwig++. Comparison between Sherpa with the CTEQ6.6 and CTEQ6L1 PDFs. New Pythia8 and PYTHIA6 tunes from ATLAS.
Greater automation of the data generation will be important, as finding resources (human rather than $\mathrm{CPU}!$ ) to produce and run combinatoric numbers of generator/tune/PDF/observable combinations has been troublesome. We suggest that this project can make use of the output of the CERN LPCC MCplots system (also Rivet-based) for future extension. We also look forward to a forthcoming major upgrade of the Rivet histogramming system which will greatly simplify the treatment of multi-leg generators for which the $n$-parton samples must be explicitly merged, e.g. AlpGen, MadGraph, etc.


## 22. COMPACT ASCII OUTPUT FORMAT FOR HEPMC 59

## Abstract

[^241]We discuss the possibility of reducing the footprint of HepMC event files. Different compression options are discussed, and a suggestion for an update of the HepMC ASCII file format is presented.

### 22.1 Introduction

The HepMC [509] event record has become the de-facto standard for communicating events between event generators and different kinds of analysis programs. HepMC also provides an ASCII-based file format for storing and retrieving events to and from disk, which has also become the standard. This file format is not at all optimized for size, and although disk space today is fairly cheap, there are still problems associated with handling very large files.
A typical minimum-bias 7 TeV LHC HepMC event occupies around 50 kB when written on disk. More interesting events are usually bigger than this and one would typically want to store many events to get anywhere near the statistics collected by any of the LHC experiments; it is clear that such event files will become very large and difficult to handle. Even with standard compression algorithms such as gzip and bzip2, where these file sizes can be reduced by a factor 3 or more, the problem is still substantial.
One could imagine using a binary output format to reduce the event size. Writing a 4 byte floating point number in an ASCII file typically takes 10-12 characters, so here one could expect to reduce file sizes up to a factor 3 . However, standard compression algorithms are rather good at identifying strings of numbers and compressing them, so there is normally not much to be gained by using a compressed binary format compared to a compressed ASCII one. In addition one would lose the advantage of ASCII files that they are (somewhat) readable to the human eye.
Instead the key to reducing file sizes is to remove redundant and unnecessary information stored in the files. This could involve completely reversible operations such as removing the information about the momentum of an intermediate particle, as this can be reconstructed from its decay products. It could also involve irreversible operations such as reducing the precision on the momenta. In the following we describe a number of such operations, which allows us to reduce the file sizes by almost a factor 30 .

### 22.2 The Benchmarking procedure

We started out by generating 1000 non-diffractive QCD events with Pythia 6.425[400] using the AGILe [360] interface. The resulting file size was 48 MB , which can be reduced to 16 MB or 13 MB using gzip or bzip2 respectively. We then investigated several ways of reducing this size.

Removing irrelevant particles The HepMC format contains quite a lot of information about how the event was generated, such as intermediate particles in the hard sub process, which may be generatordependent (and often unphysical) and is not relevant when comparing to experimental data. In principle one could argue that the only thing that should be written out is final-state stable particles (with HepMC status code 1). However, there are circumstances where information about intermediate unstable hadrons (status code 2) is relevant. The AGILe event generator interface already includes facilities for keeping only particle entries with status code 1 or 2.

Reconstructible information Some information in the HepMC file is redundant in the sense that it can be reconstructed from other information in the file. Here are some examples.

- Both energy, momentum and invariant mass of each particle is written out. Clearly, we can eg. reconstruct the energy given the three-momentum and mas $5^{60}$.

[^242]| Format | Status codes | no comp. <br> (MB) | gzip <br> (MB) | bzip2 <br> (MB) |
| :--- | ---: | ---: | ---: | ---: |
| Standard | All | 48 | 16 | 13 |
|  | $1 \& 2$ | 43 | 15 | 13 |
|  | 1 | 17 | 6.0 | 4.8 |
| Compact | All | 18 | 3.3 | 2.1 |
|  | $1 \& 2$ | 13 | 2.9 | 1.9 |
|  | 1 | 4.0 | 1.9 | 1.6 |
| Compact binary | 1 | 1.8 | 1.7 | 1.7 |

Table 18: Size of the benchmark file after applying different compression methods.

- The three-momenta of decayed hadrons (status code 2 ) can be reconstructed from the sum of the momenta of the decay products.
- The mass of a stable particle can be deduced from the particle ID.
- The position of a vertex can be deduced from the previous vertex position and the life-time and momentum direction of the connecting particle.
- Each particle in a HepMC event has a unique bar code, which is an otherwise arbitrary integer. No loss of information would result from renumbering the particles, simply inferring their bar code from the order in which they appear in the event.

Precision Clearly, having 8 byte floating point numbers is not very relevant for many of the numbers in an event file. When comparing with experimental data, there is no point in having much larger precision than what is achievable in the experiment, and it makes sense to match the the information in the HepMC file to the precision of the actually measured variables in the experiments.
A possible example is to store masses and transverse momenta as integers in units of 0.1 MeV , azimuthal angles as integers in units of $0.00002 \times \pi$, pseudorapidities as integers in units of 0.00001 and vertex positions as integers in units of 0.001 mm .

### 22.3 Benchmark Results

We have investigated several of the options listed in the previous section, and the resulting file sizes when applied to the benchmark file is presented in table 18 . Firstly we see the size reduction using the standard format and simply reducing the number of particles, keeping only those with status code 2 and 1 or only 1 . Next we present the same results, but using a compact format which keeps the structure of the HepMC ASCII file but applies all optimizations discussed above. Finally, for reference, we present an aggressively compacted Binary format which uses the following optimizations for each particle: stores 1 float for transverse and 1 float for longitudinal momentum, a 3-byte integer for phi, and 1 byte for PDG IDs (rare PDG IDs are written out with 4 full bytes). This format loses the HepMC structure of the event and in some sense this represents the target size, below which it is difficult to go.
It is clear that one does not gain much by using a binary format provided one uses the optimizations presented above together with bzip2 compression algorithm.

### 22.4 Outlook

Given the results above, the work to include a more efficient file format for the HepMC has begun. The suggestion is to keep the current structure of the file format, but to add options to exclude all particles except those with status code 1 (or 2). Furthermore options for the representation and precision of momenta and vertex positions will be included as well as options for excluding (simply replacing with a single exclamation mark for easy parsing) information which can be reconstructed. The new format will be included in a forthcoming HepMC version during 2012.

In this report we have not looked carefully at the time it takes to read the different formats. With the default HepMC format this can be many times larger than the time taken for typical particle-level analyses, while for minimal binary formats it is of the same order. We defer detailed study of this question to future work.

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# Probing gluon and heavy-quark nuclear PDFs with $\gamma+Q$ production in $p A$ collisions 

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Abstract: We present a detailed phenomenological study of direct photon production in association with a heavy-quark jet in $p A$ collisions at the Relativistic Heavy Ion Collider (RHIC) and at the Large Hadron Collider (LHC) at next-to-leading order in QCD. The dominant contribution to the cross-section comes from the gluon-heavy-quark $(g Q)$ initiated subprocess, making $\gamma+Q$ production a process very sensitive to both the gluon and the heavy-quark parton distribution functions (PDFs). Additionally, the RHIC and LHC experiments are probing complementary kinematic regions in the momentum fraction $x_{2}$ carried by the target partons. Thus, the nuclear production ratio $R_{p A}^{\gamma+Q}$ can provide strong constraints, over a broad $x$-range, on the poorly determined nuclear parton distribution functions which are extremely important for the interpretation of results in heavy-ion collisions.

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## 1 Introduction

Parton distribution functions (PDFs) are an essential component of any prediction involving colliding hadrons. The PDFs are non-perturbative objects which have to be determined from experimental input and link theoretical perturbative QCD (pQCD) predictions to observable phenomena at hadron colliders. In view of their importance, the proton PDFs have been a focus of long and dedicated global analyses performed by various groups; see e.g. refs. [1-8] for some of the most recent studies. Over the last decade, global analyses of PDFs in nuclei - or nuclear PDFs (nPDFs) - have been performed by several groups: nCTEQ [9-11], nDS [12], EKS98 [13], EPS08/EPS09 [14, 15], and HKM/HKN [16-18] (for a recent review, see ref. [19]). In a manner analogous to the proton PDFs, the nPDFs are needed in order to predict observables in proton-nucleus $(p A)$ and nucleus-nucleus $(A A)$ collisions. However, as compared to the proton case, the nuclear parton distribution functions are far less well constrained. Data that can be used in a global analysis are available for fewer hard processes and also cover a smaller kinematic range. In particular, the nuclear gluon distribution is only very weakly constrained, leading to a significant uncertainty in the theoretical predictions of hard processes in $A A$ collisions.

For this reason it is crucial to use a variety of hard processes in $p A$ collisions, both at RHIC and at LHC, in order to better constrain nuclear parton densities. The inclusive production of jets, lepton pairs or vector bosons are natural candidates since they are already used in global analyses of proton PDFs. ${ }^{1}$ In addition, other processes which could constrain the gluon nPDF have been discussed in the literature and have yet to be employed. For instance, the production of isolated direct photons [21] as well as inclusive hadrons [22] at RHIC and LHC can provide useful constraints on the nuclear gluon distribution, ${ }^{2}$ even though in the latter channel the fragmentation process complicates its extraction. Another natural candidate for measuring the gluon nPDF is heavy-quark [23] or heavy-quarkonium [24] production. Quarkonium production is however still not fully under control theoretically (see e.g. [25] for a review), hence it is not obvious whether a meaningful extraction of the nuclear gluon PDF will eventually be possible in this channel, yet indirect constraints might be obtained [26].

In this paper, we investigate the production of a direct photon in association with a heavy-quark jet in $p A$ collisions in order to constrain parton densities in nuclei. ${ }^{3}$ As we will show, this process is dominated by the heavy-quark-gluon $(Q g)$ initial state at both RHIC and the LHC making the nuclear production ratio in $p A$ over $p p$ collisions,

$$
\begin{equation*}
R_{p A}^{\gamma Q}=\frac{\sigma(p A \rightarrow \gamma Q \mathrm{X})}{A \sigma(p p \rightarrow \gamma Q \mathrm{X})}, \tag{1.1}
\end{equation*}
$$

a useful observable in order to determine the gluon and heavy-quark nPDFs in complementary $x$-ranges from RHIC to LHC. One of the advantages of such a ratio is that many of the experimental and theoretical uncertainties cancel. Nevertheless, for a solid interpretation of the ratios it is also necessary to compare the theory directly with the (differential) measured cross-sections. For this reason we present cross-sections and $p_{T}$-distributions computed at next-to-leading order (NLO) of QCD using acceptance and isolation cuts appropriate for the PHENIX and ALICE experiments at RHIC and LHC, respectively. Using the available luminosity values we also provide simple estimates for the expected event numbers.

The paper is organized as follows. In section 2 we briefly describe the NLO calculation used in the present paper (more details can be found in [28, 29]). In section 3, we discuss the different nPDF sets used in our analysis, focusing especially on the gluon and the heavyquark sectors. In sections 4 and 5 , results in $p A$ collisions at RHIC and LHC, respectively, are presented. In each case, we start with a discussion of the acceptance and isolation cuts, then turn to the (differential) cross-sections and event numbers, followed by a discussion of the nuclear production ratios. Finally, we summarize our main results in section 6 .

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## 2 Direct photon production in association with a heavy-quark jet

Single direct photons have long been considered an excellent probe of the structure of the proton due to their point-like electromagnetic coupling to quarks and due to the fact that they escape confinement [30,31]. Their study can naturally be extended to high-energy nuclear collisions where one can use direct photons to investigate the structure of nuclei as well [21].

However, it might also be relevant to study more exclusive final states, such as the double inclusive production of a direct photon in association with a heavy-quark (charm, bottom) jet ${ }^{4}$ in order to get additional constraints on parton distribution functions. The lower counting rates expected for this observable are compensated by various advantages:

- As shown below, the cross-section for direct photon plus heavy-quark production in $p p$ and $p A$ collisions is largely dominated by the gluon-heavy-quark $(g Q)$ channel. This offers in principle a direct access to the gluon and heavy-quark distributions in a proton and in nuclei;
- A two-particle final-state allows for the independent determination of the parton momentum fractions $x_{1}$ (projectile) and $x_{2}$ (target), using leading order kinematics and in the absence of fragmentation processes;
- Since the valence up quark distribution (to which single photons mostly couple) is smaller in neutrons - and therefore in nuclei - as compared to that in a proton, the nuclear production ratio $R_{p A}^{\gamma}$ of single photon production at large $x_{T}=2 p_{T} / \sqrt{s}$ is different than 1 independently of any nPDF effects [32]. In the $\gamma+Q$ production channel the photon couples mostly to the heavy-quark, which, by isospin symmetry, has the same distribution in a proton or neutron, i.e. $Q^{p}=Q^{n}$, leading to a nuclear production ratio $R_{p A}^{\gamma Q}$ free of any "isospin" effects and thus properly normalized to 1 in the absence of nPDF corrections.

At leading-order accuracy, $\mathcal{O}\left(\alpha \alpha_{s}\right)$, at the hard-scattering level the production of a direct photon with a heavy-quark jet only arises from the $g Q \rightarrow \gamma Q$ Compton scattering process, making this observable highly sensitive to both the gluon and heavy-quark PDFs. This is at variance with the single photon channel for which the Compton scattering ( $g q \rightarrow$ $\gamma q)$ as well as annihilation process $(q \bar{q} \rightarrow \gamma g)$ channels compete. ${ }^{5}$ At NLO the number of contributing subprocesses increases to seven, listed in table 1. As can be seen, all subprocesses apart from $q \bar{q} \rightarrow \gamma Q \bar{Q}$ are $g$ and/or $Q$ initiated. Which of these subprocesses dominate is highly dependent on the collider type ( $p \bar{p} v s . p p / p A$ ) and the collider center-of-mass energy. For example, $g$ and $Q$ initiated subprocesses will be more dominant at $p p$ and $p A$ colliders, whereas at the Tevatron ( $p \bar{p}$ collisions) the $q \bar{q} \rightarrow \gamma Q \bar{Q}$ dominates at high $p_{T}$ because of the valence-valence $q \bar{q}$ scattering in these collisions.

[^244]| $g g \rightarrow \gamma Q \bar{Q}$ | $g Q \rightarrow \gamma g Q$ |
| :---: | :---: |
| $Q q \rightarrow \gamma q Q$ | $Q \bar{q} \rightarrow \gamma \bar{q} Q$ |
| $Q \bar{Q} \rightarrow \gamma Q \bar{Q}$ | $Q Q \rightarrow \gamma Q Q$ |
| $q \bar{q} \rightarrow \gamma Q \bar{Q}$ |  |

Table 1. List of all $2 \rightarrow 3$ NLO hard-scattering subprocesses.

When one considers higher order subprocesses, such as $q Q \rightarrow q Q \gamma$, the produced photon may be emitted collinearly with the final state $q$ giving rise to a collinear singularity. This singular contribution is absorbed in fragmentation functions (FFs) $D_{\gamma / q}\left(z, \mu^{2}\right)$, which satisfy a set of inhomogeneous DGLAP equations, the solutions of which are of order $\mathcal{O}\left(\alpha / \alpha_{s}\right)$. As a consequence, another class of contributions of order $\mathcal{O}\left(\alpha \alpha_{s}\right)$ consists of $2 \rightarrow 2$ QCD subprocesses with at least one heavy-quark in the final state and another parton fragmenting into a collinear photon. These so-called fragmentation contributions need to be taken into account at each order in the perturbative expansion. As in the LO direct channel, we also include the $\mathcal{O}\left(\alpha \alpha_{s}^{2}\right)$ fragmentation contributions, which are needed for a complete NLO calculation. It should however be mentioned that isolation requirements - used experimentally in order to minimize background coming from hadron decays - greatly decrease these fragmentation contributions.

The present calculations have been carried out using the strong coupling constant corresponding to the chosen PDF set: $\alpha_{s}^{\overline{\mathrm{MS}}, 5}\left(M_{Z}\right)=0.118$ in next-to-leading order for both nCTEQ and EPS09, and $\alpha_{s}^{\overline{\mathrm{MS}}, 5}\left(M_{Z}\right)=0.1165$ for HKN. The renormalization, factorization and fragmentation scales have been set to $\mu_{R}=\mu_{F}=\mu_{f}=p_{T \gamma}$ and we have used $m_{c}=$ 1.3 GeV and $m_{b}=4.5 \mathrm{GeV}$ for the charm and bottom quark masses. We utilize the photon fragmentation functions of L. Bourhis, M. Fontannaz and J.P. Guillet [33]. For further details on the theoretical calculations, the reader may refer to [28, 29].

## 3 Nuclear parton distribution functions

In order to obtain results in hadronic collisions, the partonic cross-sections have to be convoluted with PDFs for protons and nuclei. For the latter we show results using the most recent nCTEQ [9, 10], EPS09 [15], and HKN07 [18] nuclear PDF sets. ${ }^{6}$ Each set of nuclear PDFs is connected to a set of proton PDFs to which it reduces in the limit $A \rightarrow 1$ where $A$ is the atomic mass number of the nucleus. ${ }^{7}$ Therefore we use the various ${ }^{n}$ PDFs together with their corresponding proton PDFs in the calculations. Since our goal is to probe gluon and heavy-quark nPDFs, let us now discuss these specific distributions in greater detail.

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Figure 1. Nuclear modifications $R_{g}^{A}=g^{p / A}(x, Q) / g^{p}(x, Q)$. Left: for gold at $Q=15 \mathrm{GeV}$. Right: for lead at $Q=50 \mathrm{GeV}$. Shown are results for nCTEQ decut3 (solid, black line), EPS09 (dashed, blue line) + error band, HKN07 (dash-dotted, red line) + error band. The boxes exemplify the $x$-regions probed at RHIC $\left(\sqrt{s_{\mathrm{NN}}}=200 \mathrm{GeV}\right)$ and the LHC $\left(\sqrt{s_{\mathrm{NN}}}=8.8 \mathrm{TeV}\right)$, respectively.

### 3.1 Gluon sector

As already mentioned, the nuclear gluon distribution is only very weakly constrained in the $x$-range $0.02 \lesssim x \lesssim 0.2$ from the $Q^{2}$-dependence of structure function ratios in deepinelastic scattering (DIS) [37], $F_{2}^{S n}\left(x, Q^{2}\right) / F_{2}^{C}\left(x, Q^{2}\right)$, measured by the NMC collaboration [38]. ${ }^{8}$

In order to compare the various nPDF sets, we plot in figure 1 the gluon distribution ratio $R_{g}^{A}(x, Q)=g^{p / A}(x, Q) / g^{p}(x, Q)$ as a function of $x$ for a gold nucleus at $Q=15 \mathrm{GeV}$ (left) and for a lead nucleus at $Q=50 \mathrm{GeV}$ (right). The chosen hard scales $Q=15,50 \mathrm{GeV}$ are typical for prompt photon production at RHIC and the LHC, respectively, and the boxes highlight the $x$-regions probed by these colliders.

As can be seen, the nuclear gluon distribution is very poorly constrained, ${ }^{9}$ especially in the regions $x<0.02$ and $x>0.1$. The uncertainty bands of the HKN07 and EPS09 gluon distributions do not overlap for a wide range of momentum fractions with $x>0.02$. Also the rather narrow and overlapping bands at small $x<0.02$ do not reflect any constraints by data, but instead are theoretical assumptions imposed on the small- $x$ behavior of the gluon distributions. The nCTEQ gluon has again quite a different $x$-shape which is considerably larger (smaller) in the $x$-region probed by RHIC (the LHC) as compared to HKN07 and EPS09.

At present, the nCTEQ nPDFs do not come with an error band. In order to assess the uncertainty of the nuclear gluon PDF we have performed a series of global fits to $\ell A$ DIS and Drell-Yan data in the same framework as described in ref. [10]. However, each time we have varied assumptions on the functional form of the gluon distribution. ${ }^{10}$ More precisely, the coefficient $c_{1}=c_{1,0}+c_{1,1}\left(1-A^{-c_{1,2}}\right)$ influencing the small $x$ behavior of the

[^246]| Name | (initial) fit parameter | $c_{1,1}$ | $c_{1,2}$ |
| :---: | :---: | :---: | :---: |
| decut3 | free | -0.29 | -0.09 |
| decut3g1 | fixed | 0.2 | 50.0 |
| decut3g2 | fixed | -0.1 | -0.15 |
| decut3g3 | fixed | 0.2 | -0.15 |
| decut3g4 | free | 0.2 | -0.15 |
| decut3g5 | fixed | 0.2 | -0.25 |
| decut3g7 | fixed | 0.2 | -0.23 |
| decut3g8 | fixed | 0.35 | -0.15 |
| decut3g9 | fixed - free proton | 0.0 | - |

Table 2. Start values for the parameter $c_{1}=c_{1,0}+c_{1,1}\left(1-A^{-c_{1,2}}\right)$ governing the small $x$ behavior of the gluon distribution at the initial scale $Q_{0}=1.3 \mathrm{GeV}$. The parameter $c_{1,0}$ corresponds to the gluon in the proton and has been kept fixed. With one exception, decut3g4, the parameters $c_{1,1}$ and $c_{1,2}$ have been kept fixed as well. For further details on the functional form the reader may refer to ref. [10].


Figure 2. Left: nPDF ratio $R_{g}^{P b}$ at $Q_{0}=1.3 \mathrm{GeV}$ predicted within the different nCTEQ sets - fits from top to bottom: decut3g9, decut3g5, decut3g7, decut3g8, decut3g3, decut3g4, decut3g2, decut3g1, decut3. Right: nCTEQ gluon nPDFs for different $\mathrm{A}(1,2,4,9,12,27$, $56,108,207)$ vs x at $Q_{0}=1.3 \mathrm{GeV}$ - from left to right, and top to bottom: decut3, decut3g1, decut3g2, decut3g3, decut3g4, decut3g5, decut3g7, decut3g8, decut3g9.
gluon distribution, see eq. (1) in [10], has been varied as summarized in table 2. Each of these fits is equally acceptable with an excellent $\chi^{2} /$ dof in the range of $\chi^{2} /$ dof $=0.88-0.9$.

In order to give an idea about the gluon nPDF uncertainty, we plot in figure 2 (left) a collection of ratios $R_{g}^{P b}$ for a lead nucleus as a function of the momentum fraction $x$ at the initial scale $Q_{0}=1.3 \mathrm{GeV}$, while in figure 2 (right) the actual gluon nPDFs are plotted versus $x$ for a range of $A$ values. Results are shown for several of the fits of the decut3g series. The ensemble of these curves together with the HKN07 and EPS09 uncertainty bands provides a much more realistic estimate of the uncertainty of the nuclear gluon distribution which is clearly underestimated by just one individual error band. This is due to the fact that for a specific fit, assumptions on the functional form of the nPDFs have


Figure 3. Nuclear modifications to deuteron, $R_{g}^{d}=g^{p / d}(x, Q) / g^{p}(x, Q)$ at $Q=15 \mathrm{GeV}$, nCTEQ (solid black line), EPS09 (dashed blue line), HKN (dash-dotted red line) + error band
been made so that the error bands based on the Hessian matrix for a given minimum only reflect the uncertainty relative to this set of assumptions.

In order to explore the allowed range of nCTEQ predictions for the nuclear production ratios to be discussed in section 4 and 5 we choose the three sets decut3 (solid black line), decut3g9 (dotted red line), and decut3g3 (dash-dotted green line). The original fit decut3 [10] exhibits a very strong shadowing at small $x$; conversely, the decut3g9 fit closely follows the distribution of the gluon in a (free) proton and the decut 3 g 3 gluon lies between the two extremes. In most cases, however, we focus on the original fit decut3 to which we refer by default as $n C T E Q$, if the fit name is not specified. Together, with the HKN07 and EPS09 predictions this will cover to a good degree the range of possibilities for the nuclear production ratios.

At RHIC, the incoming projectile is not a proton but a deuteron nucleus $(A=2)$, whose PDFs may be different from that of a proton. In figure 3 the expected nuclear modifications of the deuteron nucleus are shown. The EPS09 nPDFs do not include nuclear corrections to the deuteron PDFs, while the HKN and nCTEQ sets do. Those corrections are not large, at most $5 \%$, with nCTEQ having them more pronounced.

### 3.2 Heavy-quark sector

Let us now turn to the heavy-quark distribution. In the standard approach used in almost all global analyses of PDFs, the heavy-quark distributions are generated radiatively, according to DGLAP evolution equations [39-41], starting with a perturbatively calculable boundary condition [42, 43] at a scale of the order of the heavy-quark mass. In other words, there are no free fit parameters associated to the heavy-quark distribution and it is entirely related to the gluon distribution function at the scale of the boundary condition. As a consequence, the nuclear modifications to the radiatively generated heavy-quark PDF are very similar to those of the gluon distribution ${ }^{11}$ and quite different from the nuclear corrections in the valence-quark sector. This feature is illustrated in figure 4 (left) where

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Figure 4. Left: nPDF ratios $R_{g}^{P b}=g^{p / P b}(x, Q) / g^{p}(x, Q)$ (top), $R_{c}^{P b}=c^{p / P b}(x, Q) / c^{p}(x, Q)$ (middle), $R_{u_{v}}^{P b}=u_{v}^{p / P b}(x, Q) / u_{v}^{p}(x, Q)$ (bottom) at $Q=50 \mathrm{GeV}$ within nCTEQ (solid black line), EPS09 (dashed blue line), and HKN07 (dash-dotted red line). The shaded regions correspond to the $x$-values probed at RHIC $\left(x \sim 10^{-1}\right)$ and the LHC $\left(x \sim 10^{-2}\right)$. Right: double ratios $R_{c}^{P b} / R_{g}^{P b}$ and $R_{c}^{P b} / R_{u_{v}}^{P b}$ using the same nPDF sets.
we show the nuclear modifications for the gluon (upper panel), charm (middle panel) and the valence up-quark (bottom panel), in a lead nucleus, for three different sets of nuclear PDFs at the scale $Q=50 \mathrm{GeV}$ as in figure 1 (right). The shaded regions in figure 4 (left) correspond to the typical $x$-values probed at RHIC $\left(x \sim 10^{-1}\right)$ and the LHC $\left(x \sim 10^{-2}\right)$. The close similarity between the charm and the gluon nPDFs can be better seen in figure 4 (right) where the double ratios, $R_{c}^{P b} / R_{g}^{P b}$ and $R_{c}^{P b} / R_{u_{v}}^{P b}\left(u_{v} \equiv u-\bar{u}\right.$ being the valence distribution), are plotted. Remarkably, the nuclear effects in the gluon and the charm PDFs are different by at most $20 \%$ at large $x\left(R_{c} / R_{g} \lesssim 1.2\right)$, whereas the difference can be as large as $80 \%\left(R_{c} / R_{u_{v}} \simeq 1.8\right)$ when comparing the valence up-quark and the charm nPDF ratios. Therefore, in the standard approach, the LO direct contribution $(g Q \rightarrow \gamma Q)$ only depends on the gluon distribution, either directly or via the dynamically generated heavy-quark distribution, making this process an ideal probe of the poorly known gluon nPDF.

Conversely, light-cone models predict a nonperturbative (intrinsic) heavy-quark component in the proton wave-function [44, 45] (see [46] for an overview of different models). Recently, there have been studies investigating a possible intrinsic charm (IC) content in the context of a global analysis of proton PDFs [1, 47]. In the nuclear case, there are no global PDF studies of IC (or IB) available. This is again mainly due to the lack of nuclear data sensitive to the heavy-quark components in nuclei. For this reason, we only consider the standard radiative charm approach in the present paper. Measurements of $\gamma+Q$ production in $p A$ collisions at backward (forward) rapidities are sensitive to the BHPS-IC in nuclei (the proton) complicating the analysis. A similar statement is true for RHIC, where due to the lower center-of-mass energy the results depend on the amount of intrinsic charm. Therefore, once the nuclear gluon distribution has been better determined from other processes these cases may be useful in the future to constrain the nuclear IC.

|  | $p_{T}$ | Rapidity | $\phi$ | Isolation Cuts |
| :---: | :---: | :---: | :---: | :---: |
| Photon (+c) | $p_{T, \gamma}^{\min }=7 \mathrm{GeV}$ | $\left\|y_{\gamma}\right\|<0.35$ | $0^{\circ}<\phi<180^{\circ}$ | $R=0.5, \epsilon<0.1 E_{\gamma}$ |
| Photon (+b) | $p_{T, \gamma}^{\min }=17 \mathrm{GeV}$ | $\left\|y_{\gamma}\right\|<0.35$ | $0^{\circ}<\phi<180^{\circ}$ | $R=0.5, \epsilon<0.1 E_{\gamma}$ |
| Charm Jet | $p_{T, Q}^{\min }=5 \mathrm{GeV}$ | $\left\|y_{Q}\right\|<0.8$ | - | - |
| Bottom Jet | $p_{T, Q}^{\min }=14 \mathrm{GeV}$ | $\left\|y_{Q}\right\|<0.8$ | - | - |

Table 3. Experimental cuts used for the theoretical predictions at RHIC.


Figure 5. Differential cross-section for $\gamma+c$ (left) and $\gamma+b$ (right) production in $d$-Au collisions at a center-of-mass energy of $\sqrt{s_{\mathrm{NN}}}=200 \mathrm{GeV}$ : NLO (solid black line + band), LO (dashed blue line).

## 4 Phenomenology at RHIC

In this section we present the theoretical predictions for the associated production of a photon and a heavy-quark jet in $d$-Au collisions at RHIC at $\sqrt{s_{\mathrm{NN}}}=200 \mathrm{GeV}$.

### 4.1 Cuts

The experimental cuts used for the theoretical predictions are listed in table 3. The photon rapidity and isolation requirements are appropriate for the PHENIX detector [48]. When $p_{T, \gamma}=p_{T, Q}$ the NLO cross-section is known to become infrared sensitive. ${ }^{12}$ Therefore, in order to acquire an infrared safe cross-section, the minimum transverse momentum of the photon is kept slightly above that of the heavy-quark [49, 50] which ensures a proper cancellation between real and virtual contributions. Also note that the $p_{T}^{\min }$ cuts in the $\gamma+b$ channel $\left(p_{T, Q}^{\min }=14 \mathrm{GeV}\right.$ and $\left.p_{T, \gamma}^{\min }=17 \mathrm{GeV}\right)$ were taken to be higher than those in $\gamma+c$ events in order to keep terms of $\mathcal{O}\left(m_{Q} / p_{T}\right)$ small.

### 4.2 Spectra and expected rates

The $p_{T_{\gamma}}$ spectra are shown for $\gamma+c$ production in figure 5 (left) and $\gamma+b$ production in figure 5 (right) where the band represents the scale uncertainty obtained by varying

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Figure 6. Subprocess contributions to the differential cross-section at RHIC: NLO (solid black line), LO $+g g \rightarrow Q \bar{Q} \gamma$ (dashed blue line), $g Q \rightarrow g Q \gamma$ (dash-dotted purple line), $q \bar{q} \rightarrow Q \bar{Q} \gamma$ (dotted red line), $q(\bar{q}) Q(\bar{Q}) \rightarrow q(\bar{q}) Q(\bar{Q}) \gamma, Q Q \rightarrow Q Q \gamma$ (dash-dot-dotted magenta line).
the renormalization, factorization and fragmentation scales by a factor of two around the central scale choice, i.e., $\mu_{R}=\mu_{F}=\mu_{f}=\xi p_{T \gamma}$ with $\xi=1 / 2,2$.

The total integrated cross-section for $\gamma+c$ events is $\sigma_{\gamma+c}^{d A u}=37036 \mathrm{pb}$. Using the projected weekly luminosity for $d-A u$ collisions at RHIC-II, $\mathcal{L}^{\text {week }}=62 \mathrm{nb}^{-1}$ [51], and assuming 12 weeks of ion runs per year, the yearly luminosity is $\mathcal{L}^{y e a r}=744 \mathrm{nb}^{-1}$. Thus, an estimate of the number of events expected in one year is $N_{\gamma+c}^{d A u}=\mathcal{L}^{y e a r} \times \sigma_{\gamma+c}^{d A u} \simeq 2.8 \times 10^{4}$ in $d$-Au collisions, without taking into account effects of the experimental acceptances and efficiencies. At $p_{T_{\gamma}} \simeq 20 \mathrm{GeV}\left(\mathrm{d} \sigma / \mathrm{d} p_{T_{\gamma}} \simeq 45 \mathrm{pb} / \mathrm{GeV}\right)$, the number of events would still be large, $\mathcal{O}\left(10^{2}\right)$ per GeV -bin. This indicates that the number of $\gamma+\mathrm{c}$ events in a year produced at RHIC-II will be substantial. The rates expected in the $\gamma+b$ channel at RHIC are naturally much more modest. Using the total integrated cross-section $\sigma_{\gamma+b}^{d A u}=32 \mathrm{pb}$, the number of events to be expected in a year is $N_{\gamma+b}^{d A u}=24$. Therefore we shall mostly focus the discussion on the $\gamma+c$ channel in the following.

In figure 6 the individual subprocess contributions to the $\gamma+c$ NLO production crosssection are presented. As can be seen, the dominant subprocesses are the LO Compton scattering $g Q \rightarrow \gamma Q$, as well as the higher-order $g Q \rightarrow \gamma g Q$ and $g g \rightarrow \gamma Q \bar{Q}$ channels. Thus almost all the PDF dependence in the NLO $\gamma+c$ cross-section comes from the gluon and heavy-quark PDFs and not from the light-quark PDFs. The relative increase of the contributions by the annihilation subprocess, $q \bar{q} \rightarrow Q \bar{Q} \gamma$, and the light quark-heavy quark subprocess $q Q \rightarrow q Q \gamma$ at higher $x\left(p_{T \gamma} \sim 15 \mathrm{GeV}\right)$ is due to the slower decrease of the valence quark PDF at high $x$ as compared to the rest of the PDFs.

### 4.3 Nuclear production ratios

Let us now discuss the nuclear modifications of $\gamma+c$ production in $d$-Au collisions. The nuclear production ratio,

$$
\begin{equation*}
R_{d A u}^{\gamma+c}=\frac{1}{2 \times 197} \frac{d \sigma / d p_{T \gamma}(d \mathrm{Au} \rightarrow \gamma+c+X)}{d \sigma / d p_{T \gamma}(p p \rightarrow \gamma+c+X)}, \tag{4.1}
\end{equation*}
$$



Figure 7. Left: nuclear production ratio of the $\gamma+c$ cross-section at RHIC using nCTEQ (solid black line), nCTEQ without nuclear corrections in the deuteron (dotted magenta line), EPS09 (dashed blue line) + error band, HKN (dash-dotted red line) + error band. Right: nuclear modification of the gluon in gold, $R_{g}^{A u}\left(x, Q=x \sqrt{S} / 2 \sim p_{T}\right)$, for the $x$-region probed at RHIC. This figure corresponds to the enlargement of the box region in the left panel of figure 1.


Figure 8. Nuclear production ratio of the $\gamma+c$ cross-section at RHIC using the three nCTEQ fits discussed in section 3 . Also shown is the scale dependence of $R_{d A u}^{\gamma+c}$.
is plotted in figure 7 (left) as a function of $p_{T \gamma}$ using the three nPDF sets discussed in section 3, namely nCTEQ (solid black line), EPS09 (dashed blue line + error band) and HKN (dash-dotted red line + error band). There is some overlap between $R_{\text {HKN }}^{\gamma+c}$ and $R_{\text {EPS } 09}^{\gamma+c}$ at not too large $p_{T} \lesssim 15 \mathrm{GeV}$, whereas the difference between $R_{\mathrm{nCTEQ}}^{\gamma+c}$ on the one hand and $R_{\text {HKN }}^{\gamma+c}$ and $R_{\text {EPS09 }}^{\gamma+c}$ on the other hand is larger for all transverse momenta. The $R_{\text {nCTEQ }}^{\gamma+c}$ ratio is further increased by the anti-shadowing corrections in the deuteron projectile, as can be seen in figure 7 (left) where the nCTEQ predictions are performed with (solid line) and without (dashed) corrections in the deuteron (see also figure 3). Due to the rather low center-of-mass energy (as compared to the Tevatron/LHC) the collisions at central rapidity at RHIC probe relatively high values of momentum fractions carried by the partons in the nuclear target, $x_{2}=\mathcal{O}\left(2 p_{T} / \sqrt{s}\right)=\mathcal{O}\left(10^{-1}\right)$. In figure 7 (right) we show the nuclear modifications of the gluon distribution in a gold nucleus, $R_{g}^{A u}\left(x, Q=x \sqrt{S} / 2 \sim p_{T}\right)$, for the typical $x$-region probed at RHIC. Note that, this figure corresponds to the enlargement

|  | $p_{T}$ | Rapidity | $\phi$ | Isolation Cuts |
| :---: | :---: | :---: | :---: | :---: |
| Photon (PHOS) | $p_{T, \gamma}^{\min }=20 \mathrm{GeV}$ | $\left\|y_{\gamma}\right\|<0.12$ | $220^{\circ}<\phi<320^{\circ}$ | $R=0.2, p_{T}^{\mathrm{th}}=2 \mathrm{GeV}$ |
| Photon (EMCal) | $p_{T, \gamma}^{\min }=20 \mathrm{GeV}$ | $\left\|y_{\gamma}\right\|<0.7$ | $80^{\circ}<\phi<180^{\circ}$ | $R=0.2, p_{T}^{\mathrm{th}}=2 \mathrm{GeV}$ |
| Heavy Jet | $p_{T, Q}^{\min }=15 \mathrm{GeV}$ | $\left\|y_{Q}\right\|<0.7$ | - | - |

Table 4. Experimental cuts for the ALICE detector.
of the box-region in the left panel of figure 1. As can be seen the nuclear production ratios of $\gamma+c$ events shown in figure 7 (left) closely correspond to the different nuclear modifications of the gluon distribution depicted on the right side of figure 7. Clearly, measurements of this process with appropriately small error bars will be able to distinguish between these three different nuclear corrections to the cross-section and therefore be able to constrain the gluon nuclear PDF.

In figure 8 we present the dependence of the nuclear modifications on the three nCTEQ fits (decut3, decut3g9, decut3g3) discussed in section 3. It is clear that these different fits cover quite a spread of nuclear modifications, ranging from ones which are quite pronounced (decut3) to almost none (decut3g9). We stress again, that neither of these predictions is preferred over the other since the nuclear gluon distribution is so poorly known. Finally, we also show in figure 8 the scale uncertainty which is entirely negligible compared to the PDF uncertainty.

In the next section we present the phenomenology of $\gamma+Q$ production at the LHC where smaller values of $x_{2}$ are probed due to the higher center-of-mass energy.

## 5 Phenomenology at LHC

In this section, calculations are carried out for $p-\mathrm{Pb}$ collisions at the LHC nominal energy, $\sqrt{s_{\mathrm{NN}}}=8.8 \mathrm{TeV}$, different from the $p p$ collision energy $(\sqrt{s}=14 \mathrm{TeV})$.

### 5.1 Cuts

The cuts used in the present calculation are shown in table 4 and are appropriate for the ALICE detector ${ }^{13}$ [52-56]. Note that the rapidity shown in table 4 is given in the laboratory frame, which in $p A$ collisions is shifted by $\Delta y=-0.47$ with respect to the center-ofmass frame [57, 58]. In ALICE, photons can be identified in the EMCal electromagnetic calorimeter, or in the PHOS spectrometer with a somewhat more limited acceptance.

### 5.2 Spectra and expected rates

The differential NLO cross-section is plotted as a function of the photon transverse momentum in the $\gamma+c(\gamma+b)$ channel in figure 9 left (right) for both PHOS (lower band) and EMCal (upper band); the dotted curves indicate the theoretical scale uncertainty.

[^249]|  | $\sigma_{\gamma+Q}^{p P b}$ | $N_{\gamma+Q}^{p P b}$ |
| :---: | :---: | :---: |
| $\gamma+c$ PHOS | 22700 pb | 2270 |
| $\gamma+b$ PHOS | 3300 pb | 330 |
| $\gamma+c$ EMCal | 119000 pb | 11900 |
| $\gamma+b$ EMCal | 22700 pb | 2270 |

Table 5. Total integrated cross-section and number of events per year for $\gamma+Q$ production in $p-\mathrm{Pb}$ collisions at the LHC for PHOS and EMCal acceptances.


Figure 9. NLO differential cross-section for $\gamma+c$ (left) and $\gamma+b$ (right) production in $p-\mathrm{Pb}$ collisions at a center-of-mass energy of $\sqrt{s_{\mathrm{NN}}}=8.8 \mathrm{TeV}$ in PHOS (lower band) and EMCal (upper band) acceptances.

In order to estimate the number of events produced, we use the instantaneous luminosity $\mathcal{L}^{\text {inst }}=10^{-7} \mathrm{pb}^{-1} s^{-1}[58]$ which corresponds to a yearly integrated luminosity of $\mathcal{L}^{\text {year }}=10^{-1} \mathrm{pb}^{-1}$ assuming one month $\left(\Delta t=10^{6} s\right)$ of running in the heavy-ion mode at the LHC. In table 5 the total integrated cross-section for $\gamma+Q$ for both PHOS and EMCal along with the respective anticipated number of events (before experimental efficiencies), $N_{\gamma+Q}^{p P b}=\sigma_{\gamma+Q}^{p P b} \times \mathcal{L}^{\text {year }}$ are given. As expected the $\gamma+b$ and $\gamma+c$ cross-sections at EMCal are increased substantially by the larger acceptance of that detector. The number of expected $\gamma+b$ events is large, at variance with what is expected at RHIC (see section 4.2).

The individual subprocess contributions to the cross-section are depicted in figure 10 . As one can see the Compton $(g Q \rightarrow \gamma Q)$ as well as the $g Q \rightarrow \gamma g Q$ and $g g \rightarrow \gamma Q \bar{Q}$ are the dominant subprocesses, demonstrating the sensitivity of this process to the gluon and charm nPDFs. Here the contribution by the annihilation subprocess proves much smaller than at RHIC. This is caused by the less pronounced difference in the light anti-quark and heavy quark PDFs at small $x$ as compared to large $x$. So that now $q \bar{q} \rightarrow \gamma Q \bar{Q}$ can no longer compete with the light quark-heavy quark (antiquark) piece of the cross-section $(q Q \rightarrow q Q \gamma, q \bar{Q} \rightarrow q \bar{Q} \gamma, \bar{q} Q \rightarrow \bar{q} Q \gamma, \bar{q} \bar{Q} \rightarrow \bar{q} \bar{Q} \gamma)$.


Figure 10. Subprocess contributions to the differential cross-section shown in figure 9 (left), NLO (solid black line), LO $+g g \rightarrow Q \bar{Q} \gamma$ (dashed blue line), $g Q \rightarrow g Q \gamma$ (dash-dotted purple line), $q \bar{q} \rightarrow Q \bar{Q} \gamma$ (dotted red line), $q Q \rightarrow q Q \gamma ; Q Q \rightarrow Q Q \gamma$ (dash-dot-dotted magenta line).


Figure 11. Left: nuclear production ratio of $\gamma+c$ cross-section at LHC within ALICE PHOS acceptances, using nCTEQ decut3 (solid black line), nCTEQ decut3g3 (dotted black line), nCTEQ decut3g9 (dash-dot-dashed black line), EPS09 (dashed blue line) + error band, HKN07 (dash-dotted red line) + error band. Right: $R_{g}^{P b}\left(x, Q=x \sqrt{S} / 2 \sim p_{T}\right)$ ratio as a function of $x$, in the $x$ region probed at the LHC. This figure corresponds to the enlargement of the box region in the right panel of figure 1 .

### 5.3 Nuclear production ratios

The nuclear production ratio $R_{p P b}^{\gamma+c}=\frac{1}{208} \frac{d \sigma / d p_{T \gamma}(p \mathrm{~Pb} \rightarrow \gamma+c+X)}{d \sigma / d p_{T \gamma}(p p \rightarrow \gamma+c+X)}$ is shown in figure 11 (left) using the nCTEQ decut3 (solid black line), nCTEQ decut3g3 (dotted black line), nCTEQ decut3g9 (dash-dot-dashed black line), EPS09 (dashed blue line), and HKN07 (dashdotted red line) nuclear PDFs. For the latter two cases the bands represent the nPDF uncertainties calculated as described in section 3. Remarkably, there is almost no overlap between the EPS09 and the HKN predictions, therefore an appropriate measurement of this process will be able to distinguish between the two nPDF sets. The nCTEQ nuclear modification, using the decut3 fit, is considerably different from the two other sets at lower values of $p_{T}$. On the other hand, for the decut3g9 set, the nuclear modification factor is close to unity in the $x$-range as shown in figure 11 (right), giving rise to the nuclear pro-
duction ratio for this nCTEQ set which lies inside the EPS09 uncertainty band, figure 11 (left). We stress again that both, decut3 and decut3g9, are perfectly acceptable fits to the $\ell A$ DIS + DY data with different assumptions on the small $x$ behavior. We further show the ratio for decut3g3, as a representative lying between the two extremes. Inspecting figure 2, it is clear that the rest of the predictions from the decut3g series would fill the gap between the decut3 curve and the decut3g9 curve. Taken together, this gives a more realistic impression of the true PDF uncertainty of the nuclear production ratio. Therefore, measurements in this region will provide useful constraints on the nuclear gluon distribution.

Some further comments are in order: (i) In this paper we have demonstrated that the ratio of the $\gamma+c$ cross-section in $p A$ over $p p$ collisions at central rapidities will be very useful to constrain the nuclear gluon distribution. At forward rapidities, even smaller $x_{2}$ values could be probed in the nuclear targets where the uncertainties are largest. At backward rapidities, large $x_{2}$ is probed, hence the cross-section in this rapidity region will be sensitive to any existent intrinsic charm contribution in the nucleus. Such a measurement could be performed with the CMS and ATLAS detectors which cover a wider range in rapidity. We postpone such a study to a future publication, since currently there are no available IC nuclear PDFs; (ii) At the LHC $\gamma+b$ events will also be produced with sufficient statistics. Experimentally this channel might be preferable due to the much better $b$-tagging efficiencies. Furthermore, uncertainties related to possible intrinsic charm contributions should be much reduced in the bottom case. However, as for $\gamma+c$ production, the nuclear production ratios follow closely the gluon ratio and, therefore, we do not show a separate figure here.

## 6 Conclusions

We have performed a detailed phenomenological study of direct photon production in association with a heavy-quark jet in $p A$ collisions at RHIC and at the LHC, at next-to-leading order in QCD. The dominant contribution to this process is given by the $g Q \rightarrow \gamma Q[+g]$ subprocess. This offers a sensitive mechanism to constrain the heavy-quark and gluon distributions in nuclei, whose precise knowledge is necessary in order to predict the rates of hard processes in heavy-ion collisions where quark-gluon plasma is expected to be formed.

We have performed the calculation of $\gamma+Q$ production spectra at RHIC and at the LHC within the acceptances of various detectors (PHENIX and ALICE-PHOS/ALICE-EMCal) and have presented the corresponding counting rates. At the LHC the $\gamma+c$ and $\gamma+b$ production rate is important, while at RHIC only $\gamma+c$ events will be copiously produced.

Our results for RHIC (see figure 7) exhibit a strong sensitivity to the nuclear gluon distribution permitting to constrain it at $x \sim 0.1-0.2$. Similarly to RHIC the ratio at the LHC (see figure 11) is very sensitive to the gluon distribution probing a smaller $x \sim 10^{-2}$, i.e. in a complementary range to RHIC . These results have been obtained in the "standard approach" of radiatively generated charm distribution. A future study will focus on the possibility to constrain the intrinsic charm contribution to the nucleus as well as the proton.

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# Constraints on color-octet fermions from a global parton distribution analysis 

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#### Abstract

We report a parton distribution function analysis of a complete set of hadron scattering data, in which a color-octet fermion (such as a gluino of supersymmetry) is incorporated as an extra parton constituent along with the usual standard model constituents. The data set includes the most up-to-date results from deep inelastic scattering and from jet production in hadron collisions. Another feature is the inclusion in the fit of data from determinations of the strong coupling $\alpha_{s}(Q)$ at large and small values of the hard scale $Q$. Our motivation is to determine the extent to which the global parton distribution function analysis may provide constraints on the new fermion, as a function of its mass and $\alpha_{s}\left(M_{Z}\right)$, independent of assumptions such as the mechanism of gluino decays. Based on this analysis, we find that gluino masses as low as 30 to 50 GeV may be compatible with the current hadronic data. Gluino masses below $15 \mathrm{GeV}(25 \mathrm{GeV})$ are excluded if $\alpha_{s}\left(M_{Z}\right)$ varies freely (is equal to 0.118 ). At the outset, stronger constraints had been anticipated from jet production cross sections, but experimental systematic uncertainties, particularly in normalization, reduce the discriminating power of these data.


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## I. INTRODUCTION

Heavy color-octet particles are postulated in theories of beyond-the-standard-model (BSM) phenomena, including supersymmetry (SUSY) [1], universal extra dimensions [2], Randall-Sundrum [3], and Little Higgs models [4]. Direct searches for such states are usually guided by aspects of the production and decay dynamics in the particular BSM approach. Analyses of search data have so far produced various bounds on the masses of the states, often conditioned by model-dependent assumptions [5-15]. Different constraints, such as the SUSY gluino mass bounds $m_{\tilde{g}}>$ 26.9 GeV [16] and 51 GeV [17] at $95 \%$ confidence level (C.L.), are based on the analysis of LEP event shapes in soft-collinear effective theory and other quantum chromodynamics (QCD) resummation formalisms. Constraints such as these may depend on theoretical modeling of nonperturbative hadronization and the matching of hard scattering and resummed contributions, similar to the determination of $\alpha_{s}\left(M_{Z}\right)$ from LEP data in QCD [18-22]. In a previous publication [23], we examine the possibility that a global analysis of hadron data, within the framework of parton distribution function (PDF) determinations, can be used to derive constraints on the existence and masses of color-octet fermions, independently of other information on such states. Global analysis has discriminating power for several reasons: one is that new colored states modify the evolution with hard scale $Q$ of the strong coupling strength $\alpha_{s}(Q)$. Second, in perturbative QCD , the coupling of a color-octet fermion to quarks and gluons alters the set of evolution equations that governs the behavior of all parton distribution functions, thus affecting many hadron scattering cross sections. Moreover, production of the color-octet
states will affect relevant observables, such as jet rates, whose cross sections are included in the global fits.

The specific case of a gluino from supersymmetry is included as an extra degree of freedom in our earlier work [23]. We refer to the PDFs obtained in that publication as "SUSY PDFs," although our analysis is applicable to a broader class of standard model (SM) extensions. In Ref. [23], a lower bound on the gluino mass $m_{\tilde{g}}$ is obtained in terms of an assumed value of $\alpha_{s}\left(M_{Z}\right)$ at $Z$ boson mass $M_{Z}$. For the then standard model world-average value of $\alpha_{s}\left(M_{Z}\right)=0.118$, gluinos lighter than 12 GeV were shown to be disfavored, whereas the lower bound was relaxed to less than 10 GeV (less than 2 GeV ) when $\alpha_{s}\left(M_{Z}\right)$ was increased above 0.120 ( 0.127 ).

In this paper, we use new hadron scattering data incorporated in the next-to-leading order (NLO) CT10 generalpurpose PDF analysis [24], along with a new approach for incorporating the variation of $\alpha_{s}(Q)$ into PDF determinations [25], to obtain improved bounds on the mass of a relatively light gluino. The essential new elements are these:
(i) New Tevatron jet data [26-28] and combined DIS data [29] from HERA. In a global QCD analysis, the presence of light gluinos is revealed primarily by modifications of $\alpha_{s}\left(M_{Z}\right)$, the gluon PDFs, and the charm and bottom quark PDFs, generated radiatively above the respective heavy-quark thresholds. We include the latest hadronic scattering data sensitive to such modifications. The most stringent constraints on the gluon PDF are imposed by electron-proton deep inelastic scattering (DIS) data at $x<0.1$ and single-inclusive jet production data from the Tevatron $p \bar{p}$ collider at $x \gtrsim 0.1$. The study reported
here incorporates up-to-date information from the combined H1 Collaboration and ZEUS Collaboration data on deep inelastic scattering at HERA-1 [29], as well as single-inclusive jet data from the Tevatron Run-II analyses [26-28]. Hard scattering contributions of massive gluinos, with full dependence on the gluino's mass, are included in the jet production cross sections we use, the only process we examine where these contributions are large enough to be relevant at NLO accuracy.
(ii) Floating $\alpha_{s}\left(M_{Z}\right)$. Our fits are performed by treating $\alpha_{s}\left(M_{Z}\right)$ at the mass $M_{Z}$ of the $Z$ boson as a variable parameter of the standard model. We constrain $\alpha_{s}\left(M_{Z}\right)$ by requiring that the fitted $\alpha_{s}(Q)$ agree with its direct determinations at low-energy scales $(Q<10 \mathrm{GeV})$ and at $Q=M_{Z}$, within the quoted uncertainties of these measurements. Virtual gluino contributions result in a slower evolution of the QCD coupling strength $\alpha_{s}(Q)$ at scales $Q$ above the gluino mass threshold. By including data that constrain $\alpha_{s}$ at low and high $Q$ scales, we effectively probe for deviations from pure QCD. We find, in particular, that the value of $\alpha_{s}\left(M_{Z}\right)=0.123 \pm$ 0.004 derived in some analyses of LEP event shapes [20] can be accommodated if gluinos have mass of about 50 GeV .
The remainder of this paper is organized as follows. In Sec. II, we describe the role of new color-octet fermions in a global QCD analysis. The incorporation of data on $\alpha_{s}(Q)$ within the global fits is discussed in Sec. III, where we also present the values of $\alpha_{s}(Q)$ at high and low $Q$ used in our fits. Our simultaneous global fit to hadronic scattering data and $\alpha_{s}(Q)$ is described in Sec. IV, where we also examine the effects of an additional gluino degree of freedom on the PDFs. We present figures that show the relative magnitudes of the PDFs and the variation of their momentum fractions with gluino mass and hard scale.

Section V contains the results of our detailed comparison with data. We present figures that show the variation of the values of $\chi^{2}$ in the global analyses, as a function of gluino mass, for both floating and fixed $\alpha_{s}\left(M_{Z}\right)$. Section V also includes the comparison of our calculated cross sections with jet data from the Tevatron collider and a discussion of the systematic uncertainties that limit the constraining power of these data. The sensitivity of jet cross sections at the LHC to the presence of gluinos is examined in Sec. VI. Our conclusions are presented in Sec. VII. The appendices contain an analytic expression for the evolution of the strong coupling $\alpha_{s}(Q)$ in terms of the SM and SUSY degrees of freedom, expressions for the contributions of massive gluinos to the jet production cross sections, and parton-parton luminosity functions for various combinations of SM partons and gluinos.

Based on our analysis, we conclude that gluino masses as low as 30 to 50 GeV may be compatible with the current
hadronic data, depending on the value of $\alpha_{s}\left(M_{Z}\right)$. For a floating $\alpha_{s}\left(M_{Z}\right)$, gluinos lighter than 15 GeV are excluded. For an assumed fixed value $\alpha_{s}\left(M_{Z}\right)=0.118$, the worldaverage value used in many phenomenological analyses, gluinos lighter than 25 GeV , are disfavored.

We acknowledge that a gluino as light as $\sim 50 \mathrm{GeV}$ is not typical in phenomenological models of SUSY breaking, nor of the results of experimental direct search analyses based on specific models of SUSY breaking and assumptions about mass relationships among SUSY states [15]. As long as the SUSY neutralino $\tilde{\chi}^{0}$ is lighter than the gluino, the typical decay process for a light gluino is $\tilde{g} \rightarrow$ $q \bar{q} \tilde{\chi}^{0}$, where $q$ stands for a SM quark. Missing energy would signal the presence of a neutralino. However, for a small mass splitting $m_{\tilde{g}}-m_{\tilde{\chi}^{0}}$, the gluino's decay into missing energy and soft quark jets would be undetected. The analysis reported here is complementary to other approaches for bounding the gluino mass, and it is in some respects more general in that we make no assumptions about the gluino decay.

Precise determination of $\alpha_{s}\left(M_{Z}\right)$ and proton PDFs are essential ingredients for obtaining reliable predictions from perturbative QCD calculations. Such calculations are key for the general physics program and for new physics searches at the CERN Large Hadron Collider (LHC) and Fermilab Tevatron collider. As we show here, these ingredients themselves may be affected by non-SM contributions, at all values of the momentum fraction $x$, as a result of the global interconnections in PDF analyses. The determination of the QCD coupling $\alpha_{s}$ and of the gluon PDF from the Tevatron or LHC single-inclusive jet data, such as in recent Tevatron Run-2 measurements [26-28,30], may be sensitive to scattering of color-octet fermions in the ways discussed in Sec. VI. As a result of our work, we determine new sets of PDFs that include a relatively light gluino as a hadron constituent.

## II. COLOR-OCTET FERMIONS IN A GLOBAL QCD ANALYSIS

Under well-defined conditions, a relatively light strongly-interacting fundamental particle may be treated as a constituent of the colliding hadrons. It will share the momentum of the parent hadron with the standard model quark, antiquark, and gluon partners. The experimental consequences of this picture become evident when the parent hadron is probed at a sufficiently large hard scale. For example, the charm quark $c$ and bottom quark $b$ are treated appropriately as partonic constituents of hadrons when the characteristic energy scale $Q$ exceeds the mass of the heavy quark $m_{q}$. Likewise, when $Q$ greatly exceeds the mass of a new strongly-interacting particle, this object must also be incorporated as a hadronic constituent. We refer to Ref. [23] for an exposition of the PDF analysis in which a gluino is included as an additional partonic degree of freedom.


FIG. 1. LO scattering diagrams in inclusive jet production with gluinos in the initial or final state. The double lines stand for the squark exchange contributions that we neglect in our approximation.

As in Ref. [23], we take the gluino as the only colored non-SM degree of freedom that needs to be considered. In some models of SUSY breaking, such as split supersymmetry [31,32], the squarks are much heavier than the gluinos, and therefore could be omitted from our PDF analysis. Moreover, as illustrated in Eq. (A3) of Appendix A, color-octet spin- $1 / 2$ fermions have a greater impact on the evolution of the strong coupling $\alpha_{s}$ than color triplet scalars, such as squarks. ${ }^{1}$

The presence of a light gluino $\tilde{g}$ modifies the PDF global analysis in three ways.
(1) The gluino changes the evolution of the strong coupling strength $\alpha_{s}(Q)$, as the scale $Q$ is varied. This influence is implemented in our results, and we provide details on the running of $\alpha_{s}(Q)$ in Appendix A. The constraints on the gluino mass from our global analysis depend significantly on the value of the strong coupling strength $\alpha_{s}\left(M_{Z}\right)$.
(2) The gluino provides an additional partonic degree of freedom that shares in the nucleon's momentum. It alters the coupled set of Dokshitzer-Gribov-Lipatov-Altarelli-Parisi equations that govern the evolution of the parton distributions,

$$
\begin{align*}
Q^{2} \frac{d}{d Q^{2}}\left(\begin{array}{c}
\Sigma(x, Q) \\
g(x, Q) \\
\tilde{g}(x, Q)
\end{array}\right) & =\frac{\alpha_{s}(Q)}{2 \pi} \times \int_{x}^{1} \frac{d y}{y}\left(\begin{array}{ccc}
P_{\Sigma \Sigma}^{\mathrm{NLO}}(x / y) & P_{\Sigma g}^{\mathrm{NLO}}(x / y) & P_{\Sigma \tilde{g}}^{\mathrm{LO}}(x / y) \\
P_{g \Sigma}^{\mathrm{NLO}}(x / y) & P_{g g}^{\mathrm{NL}}(x / y) & P_{g \tilde{\mathrm{~L}}}^{\mathrm{L}}(x / y) \\
P_{\tilde{g} \Sigma}^{\mathrm{LO}}(x / y) & P_{\tilde{g} g}^{\mathrm{LO}}(x / y) & P_{\tilde{g} \tilde{g}}^{\mathrm{L}}(x / y)
\end{array}\right)\left(\begin{array}{c}
\Sigma(y, Q) \\
g(y, Q) \\
\tilde{g}(y, Q)
\end{array}\right) ; \\
\Sigma(x, Q) & =\sum_{i=u, d, s, \ldots}\left(q_{i}(x, Q)+\bar{q}_{i}(x, Q)\right) . \tag{1}
\end{align*}
$$

Here $\Sigma(x, Q), g(x, Q)$, and $\tilde{g}(x, Q)$ are the singlet quark, gluon, and gluino distributions, respectively; $q_{i}(x, Q)$ and $\bar{q}_{i}(x, Q)$ are the quark and antiquark distributions for a flavor $i$. The previous analysis [23] shows that the gluino's contribution is small in the momentum fraction range $x>10^{-5}, \tilde{g}(x, Q) \ll$ $g(x, Q)$, and $\tilde{g}(x, Q) \ll q(x, Q)$. NLO variations in the relevant SUSY cross sections are small and comparable in size to variations associated with next-to-next-to-leading order (NNLO) SM contributions. Therefore, the leading-order (LO) approximation for the splitting functions and hard scattering amplitudes of SUSY terms is numerically adequate, when combined with NLO expressions for SM contributions.
(3) At energies above its mass threshold, a color-octet fermion contributes to hard scattering processes as

[^250]an incident parton and/or as a produced particle. However, as argued in Ref. [23], in the absence of light squarks, gluino hard scattering contributions to DIS and Drell-Yan process are of next-to-next-toleading order and negligible in the current study. At the same time, the hard scattering gluino terms contribute at the LO in single-inclusive jet production, so that it is essential that we include the gluino in the corresponding hard scattering matrix elements of jet cross sections.
The $2 \rightarrow 2$ hard scattering contributions with two gluinos in the initial or final states are illustrated in Fig. 1. We assume that the masses of the squarks are large enough that diagrams containing a squark propagator are negligible. The remaining SUSY diagrams can be evaluated in the the S-ACOT factorization scheme $[34,35]$, in order to simplify treatment of the gluino mass dependence. In this scheme, gluino mass terms are retained in diagrams with two final-state gluinos in the subprocesses $g g \rightarrow \tilde{g} \tilde{g}$ and $q \bar{q} \rightarrow \tilde{g} \tilde{g}$. Explicit scattering amplitudes in these
channels are documented in Eqs. (B2) and (B3) of Appendix B. Massless amplitudes are used for the remaining $2 \rightarrow 2$ hard scattering subprocesses, in which one or two gluinos are present in the initial state, and whose contributions are proportional to the gluino PDF $\tilde{g}(x, Q)$. This arrangement captures the full gluino mass dependence, while including the mass terms only in the essential scattering amplitudes.

## III. QCD COUPLING STRENGTH AS A FITTING PARAMETER

Since the range of $m_{\tilde{g}}$ values allowed by the global fits depends strongly on the assumed value of $\alpha_{s}\left(M_{Z}\right)$, we do a simultaneous fit to hadronic data and to data on $\alpha_{s}(Q)$ in this work. A judicious choice is required therefore of the set of data on $\alpha_{s}(Q)$.

Our approach is to fit the global set of data using $\alpha_{s}(Q)$ as a floating parameter, constraining it with additional data on $\alpha_{s}(Q)$ measurements at $Q<10 \mathrm{GeV}$ (i.e., in the range where gluino contributions are excluded by the previous analysis), and at $Q=M_{Z}$ (in $e^{+} e^{-}$hadroproduction at LEP). This approach is similar to the floating $\alpha_{s}\left(M_{Z}\right)$ fit in Ref. [25]. However, we constrain $\alpha_{s}(Q)$ at two distinct $Q$ values, to probe for deviations of its running from the SM prediction.

## A. Low-energy constraints

The QCD coupling constraint at low $Q=5 \mathrm{GeV}$,

$$
\begin{equation*}
\alpha_{s}(Q=5 \mathrm{GeV})=0.213 \pm 0.002 \tag{2}
\end{equation*}
$$

is obtained as a weighted average of three precise determinations of $\alpha_{s}$ at comparable energies:

$$
\begin{gather*}
\alpha_{s}(Q=5 \mathrm{GeV})=0.219 \pm 0.006 \text { from } \tau \text { decays }  \tag{3}\\
\alpha_{s}(Q=5 \mathrm{GeV})=0.214 \pm 0.003  \tag{4}\\
\text { from heavy quarkonia, } \\
\alpha_{s}(Q=5 \mathrm{GeV})=0.209 \pm 0.004 \text { from lattice } \mathrm{QCD} \tag{5}
\end{gather*}
$$

These values are reconstructed by QCD evolution to the common scale $Q=5 \mathrm{GeV}$ of the published $\alpha_{s}$ values provided at different energy scales,

$$
\begin{gather*}
\left(\alpha_{s}\right)_{\tau}=0.330 \pm 0.014 \quad \text { at } m_{\tau}=1.77 \mathrm{GeV}  \tag{6}\\
\left(\alpha_{s}\right)_{Q \bar{Q}}=0.1923 \pm 0.0024 \text { at } M_{Q \bar{Q}}=7.5 \mathrm{GeV}  \tag{7}\\
\left(\alpha_{s}\right)_{\text {lattice }}=0.1170 \pm 0.0012 \text { at } M_{Z}=91.18 \mathrm{GeV} \tag{8}
\end{gather*}
$$

The value of $\left(\alpha_{s}\right)_{\tau}$ is determined from measurements of $\tau$ decays [36], $\left(\alpha_{s}\right)_{Q \bar{Q}}$ comes from heavy-quarkonium decays [37], and $\left(\alpha_{s}\right)_{\text {lattice }}$ is obtained from lattice computations [37].

The $\tau$ decay and heavy-quarkonium determinations of $\alpha_{s}$ can be reasonably assumed to be independent of gluino effects. Even if very light gluinos $(\approx 10 \mathrm{GeV})$ were present, the value of $\alpha_{s}$ in these measurements would not be affected. The lattice QCD value $\left(\alpha_{s}\right)_{\text {lattice }}$ is also determined at $Q<10 \mathrm{GeV}$ from the energy levels of heavy quarkonia [37], and then evolved by the authors to $Q=M_{Z}$ assuming the $\mathrm{SM} \beta$ function. We reconstruct the "directly measured" lattice QCD value at $Q=5 \mathrm{GeV}$ (independent of the gluino effects) by backward SM evolution. We then combine the lattice QCD value with the other two low- $Q$ measurements, evolved to the same scale using the $\operatorname{SM} \beta$ function, to obtain a composite data input to the fit.

## B. $Z$ pole constraints

If $m_{\tilde{g}}<M_{Z}$, the value of $\alpha_{s}\left(M_{Z}\right)$ extracted from the LEP $e^{+} e^{-}$hadroproduction data could differ from the value obtained from SM fits. On the other hand, various determinations of $\alpha_{s}\left(M_{Z}\right)$ from $Z$ boson width and hadronic event shapes [18-22,38] show no obvious need for BSM contributions. Thus, if gluinos are lighter than $Z$ bosons, their contributions to the LEP observables are of the order of theoretical uncertainties from other sources. Notably related to assumptions about nonperturbative hadronization in LEP observables, these uncertainties remain substantial and produce central values of $\alpha_{s}\left(M_{Z}\right)$ ranging from 0.1135 [21,22] to 0.1224 [20]. To deal with this issue of choice, one solution is to include available values of $\alpha_{s}\left(M_{Z}\right)$ derived from the $Z$ width and/or event shape measurements, assuming that gluino contributions for these measurements are comparable with the current experimental plus theoretical uncertainties.


FIG. 2 (color online). Running of the strong coupling as a function of the scale $Q$. The red solid line represents the SM evolution, while the dashed lines are plotted for $m_{\tilde{g}}=50,25,10$, 5 GeV . The points with the error bands represent the low- $Q$ and high- $Q$ constraints, given in Eqs. (2) and (9), respectively.

Absent a gluino lighter than the $Z$ boson (i.e., if only SM particles contribute at $Q<M_{Z}$ ), NLO evolution of the composite low- $Q$ value in Eq. (2) to the $Z$ pole results in $\alpha_{s}\left(M_{Z}\right)$ close to 0.118 . Global analysis of hadronic scattering alone also leads to a preferred value $\alpha_{s}\left(M_{Z}\right)=$ $0.118 \pm 0.005$ at $90 \%$ C.L., cf. recent CTEQ fits [25].

If the gluino is lighter than $M_{Z}$, the resulting evolved value at $Q=M_{Z}$ is higher. For example, the evolved $\alpha_{s}\left(M_{Z}\right)$ is 0.126 or 0.121 , if $m_{\tilde{g}}$ is 20 or 50 GeV . This variation is illustrated in Fig. 2, showing the dependence of $\alpha_{s}(Q)$ on the scale $Q$ in the absence of light gluinos (solid line) and with gluinos of mass $m_{\tilde{g}}=50,25,10$, and 5 GeV . In the figure, we show the low- $Q$ constraint (the left data point), as well as one of available constraints at the $Z$ pole, $\alpha_{s}\left(M_{Z}\right)=0.123 \pm 0.004$ [20]. As seen in the figure, a light gluino with a mass of $m_{\tilde{g}}=10 \mathrm{GeV}$ cannot simultaneously accommodate the low- $Q$ and high- $Q$ constraints. On the other hand, gluinos with mass about 50 GeV are compatible with both constraints, and are even preferred if the high- $Q$ constraint on $\alpha_{s}$ is larger than 0.118 .

To illustrate typical possibilities, we therefore present two kinds of fits in this paper: one in which a fixed value of $\alpha_{s}\left(M_{Z}\right)=0.118$ is assumed, and the other in which $\alpha_{s}\left(M_{Z}\right)$ varies and is constrained by an assumed high- $Q$ data point,

$$
\begin{equation*}
\alpha_{s}\left(M_{Z}\right)=0.123 \pm 0.004 \tag{9}
\end{equation*}
$$

compatible with [20].

## C. Log-likelihood function for coupling strength constraints

With the additional constraints on the running coupling, the total log-likelihood function $\chi_{\text {tot }}^{2}$ is

$$
\begin{equation*}
\chi_{\mathrm{tot}}^{2}=\chi_{\text {h.s. }}^{2}+\chi_{\alpha_{s}}^{2}, \tag{10}
\end{equation*}
$$

where $\chi_{\text {h.s. }}^{2}$ is the $\chi^{2}$ contribution of the hadron scattering (h.s.) experiments, i.e., DIS, vector boson production, and jet production; $\chi_{\alpha_{s}}^{2}$ is the contribution from the direct constraints on $\alpha_{s}$ :

$$
\begin{equation*}
\chi_{\alpha_{s}}^{2}=\lambda \sum_{i=1}^{N_{\alpha_{s}}}\left(\frac{\left.\alpha_{s}^{(i)}\right|_{\exp }-\left.\alpha_{s}^{(i)}\right|_{\mathrm{th}}}{\left.\delta \alpha_{s}^{(i)}\right|_{\exp }}\right)^{2} \tag{11}
\end{equation*}
$$

In this equation, $N_{\alpha_{s}}$ is the number of data points constraining $\alpha_{s} ; N_{\alpha_{s}}=2$ in our case. $\left.\alpha_{s}^{(i)}\right|_{\text {exp }}$ and $\left.\delta \alpha_{s}^{(i)}\right|_{\text {exp }}$ are the central value and error of the experimental measurements in Eqs. (2) and (9); $\left.\alpha_{s}^{(i)}\right|_{\text {th }}$ are the respective two-loop theoretical values. We assume that an increase in $\chi^{2}$ by 100 units above the best-fit value corresponds to approximately $90 \%$ C.L. error, in accordance with the convention of the previous CTEQ6 analysis [39] and 2004 gluino study [23]. To match this convention, the $\alpha_{s}$ contribution $\chi_{\alpha_{s}}^{2}$ is included with a factor $\lambda=37.7$, so that a deviation of $\left.\alpha_{s}^{(i)}\right|_{\text {th }}$ by $\left.1.6 \delta \alpha_{s}^{(i)}\right|_{\exp }$ ( $90 \%$ C.L.) corresponds to $\Delta \chi_{\alpha_{s}}^{2} \approx 100$.

## IV. GLOBAL FITS

In this section we describe our simultaneous global fit to hadronic scattering data and $\alpha_{s}(Q)$, and we examine the effects of an additional gluino degree of freedom on the PDFs.

Our SUSY fits include the same set of data as the latest CT10 fit of parton distributions [24]. A total of 2753 data points from 35 experiments is included. Besides the data studied in the previous CTEQ6.6 analysis [40], the new analysis includes the combined DIS data from HERA-1 [29] and single-inclusive jet data from the Tevatron Run-2 analyses [26-28]. The new data provide important constraints on the gluon PDF, the parton density that is most affected by the gluinos. The charm and bottom PDFs are also affected, since they are generated by DGLAP evolution from the gluon PDF above the initial scale $Q_{0}=m_{c}=$ 1.3 GeV .

The ratios of the best-fit gluon and charm PDFs in the SUSY sets to their counterparts in the standard model CT10 set, $f_{\text {SUSY }}(x, Q) / f_{\text {CT10 }}(x, Q)$, are shown as dashed curves in Figs. 3 and 4, at $Q=2$ and 85 GeV , for two values of the gluino mass, $m_{\tilde{g}}=20$ and 50 GeV . The normalized CT10 uncertainty bands are shown also, defined as

$$
\begin{equation*}
\frac{f_{\mathrm{CT} 10}(x, Q) \pm \delta_{ \pm} f_{\mathrm{CT} 10}(x, Q)}{f_{\mathrm{CT} 10}(x, Q)} \tag{12}
\end{equation*}
$$

in terms of asymmetric PDF uncertainties $\delta_{ \pm} f_{\mathrm{CT} 10}(x, Q)$ [24,41]. Figure 3 pertains to fits with a floating $\alpha_{s}\left(M_{Z}\right)$, whereas Fig. 4 is based on a fixed $\alpha_{s}\left(M_{Z}\right)=0.118$.

If $\alpha_{s}\left(M_{Z}\right)$ varies (Fig. 3), modifications in the gluon distribution are moderate at most. Some differences with the CT10 predictions are observed at large $x$, notably in the range $x>0.01$ in $g(x, Q)$ at $Q=85 \mathrm{GeV}$ and in $c(x, Q)$ at $Q=2 \mathrm{GeV}$. The difference is larger for a lighter gluino with $m_{\tilde{g}}=20 \mathrm{GeV}$. Other PDFs exhibit smaller differences, all contained in the standard model uncertainty band.

For a fixed $\alpha_{s}\left(M_{Z}\right)=0.118$ (Fig. 4), the differences with CT10 are substantial. At $Q=2 \mathrm{GeV}$, the SUSY PDFs lie outside of CT10 error bands for $x$ as low as $10^{-3}$. At $Q=85 \mathrm{GeV}$, the difference persists at $x>$ $0.01-0.05$. Large differences between the SUSY and CT10 PDF's in the case of a fixed strong coupling are attributed to sizable deviations from SM running of $\alpha_{s}$ and compensating adjustments in $g(x, Q)$ observed for relatively light gluinos; cf. Figs. 12b and 5 in Ref. [23].

The effect of the gluino on the standard model quark and gluon PDFs can be significant, even if $m_{\tilde{g}}$ is large compared to $m_{c}$ and $m_{b} .{ }^{2}$ Because the gluino is an active

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FIG. 3 (color online). Ratios of $g(x, Q)$ (upper row) and $c(x, Q)$ (lower row) distributions in SUSY fits with floating $\alpha_{s}\left(M_{Z}\right)$ and the CT10 fit at $Q=2 \mathrm{GeV}$ (left) and $Q=85 \mathrm{GeV}$ (right), for the gluino mass $m_{\tilde{g}}$ of 20 and 50 GeV .
constituent of the proton, it carries a finite momentum fraction, taken from the other non-SUSY partons, primarily the gluon. This feature is evident in Table I where we display the partonic momentum fractions for gluino masses $m_{\tilde{g}}=\{20,50,100\} \mathrm{GeV}$.

Gluinos draw most of their momentum fraction from the gluon, since the primary coupling is via the process $g \rightarrow$ $\tilde{g} \tilde{g}$. The influence on the quarks is a second-order effect transmitted through the gluon. At $Q=100 \mathrm{GeV}$, the momentum fraction of the lighter gluinos $\left(m_{\tilde{g}} \sim 20 \mathrm{GeV}\right)$ is comparable to that of the strange quark, even though the gluino mass is an order of magnitude larger. For $m_{\tilde{g}} \sim$ 50 GeV , the momentum fraction of the gluino is comparable to that of the bottom quark. The magnified impact of the gluino on the QCD evolution, compared to the usual quark flavors, can be understood from a comparison of the $g \rightarrow \tilde{g}$ splitting kernel,

$$
\begin{equation*}
P_{g \rightarrow \tilde{g}}(x)=3\left[(1-x)^{2}+x^{2}\right] \tag{13}
\end{equation*}
$$

with the usual gluon-quark splitting function

$$
\begin{equation*}
P_{g \rightarrow q}(x)=\frac{1}{2}\left[(1-x)^{2}+x^{2}\right] . \tag{14}
\end{equation*}
$$

The effect of the gluino as a hadronic constituent in the QCD evolution is thus equivalent to that of 6 quark flavors, $P_{g \rightarrow \tilde{g}}=6 P_{g \rightarrow q}$.

As an illustration of the relative magnitude of the gluino PDF, Fig. 5 displays PDFs for various parton flavors as a function of $x$ for our $m_{\tilde{g}}=50 \mathrm{GeV}$ PDF set and a hard scale of $Q=100 \mathrm{GeV}$. At $x>0.001$, the gluino PDF is about equal to the bottom quark PDF, the smallest of the quark PDFs. For smaller $x$, it grows in magnitude and catches up with the other quark PDFs at $x=10^{-5}$, as a consequence of its faster DGLAP evolution. Parton-parton luminosities dependent on the gluino PDF, useful for computations of cross sections, are plotted in Appendix C.

## V. COMPARISON OF THEORY AND DATA

In this section, we show the results of our global fits, the constraints we obtain on the mass of a gluino, and the impact of a gluino degree of freedom on the analysis of jet data.


FIG. 4 (color online). Same as Fig. 3, but for a fixed $\alpha_{s}\left(M_{Z}\right)=0.118$.

The figures in the previous section show that the SM +SUSY PDFs disagree with CT10 PDFs if gluinos are lighter than 20 GeV , indicating that the SM+SUSY PDFs for these gluino masses cannot describe the global hadronic data well. Gluinos with somewhat larger masses can be accommodated, or may be slightly preferred to the pure SM case, depending on the value of $\alpha_{s}\left(M_{Z}\right)$. These points are illustrated in a different way by the summary of values of $\chi^{2}$ in Table II, for $m_{\tilde{g}}=10,20$, and 50 GeV , as well as for the standard model case (equivalent to $m_{\tilde{g}}=\infty$ ). The

TABLE I. Momentum fraction $F_{i}=\int_{0}^{1} d x x f_{i}(x, Q)$ for each partonic flavor $i$ at scale $Q=100 \mathrm{GeV}$. Momentum fractions for $\{\bar{s}, \bar{c}, \bar{b}\}$ are not shown and must be included to satisfy the sum rule.

| Momentum fractions for $Q=100 \mathrm{GeV}$ in percent |  |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $m_{\tilde{g}}[\mathrm{GeV}]$ | $\tilde{g}$ | $d$ | $\bar{u}$ | $g$ | $u$ | $d$ | $s$ | c | $b$ |
| 20 | 2.8 | 3.9 | 3.4 | 44.3 | 21.8 | 11.4 | 3.0 | 1.8 | 1.2 |
| 50 | 1.2 | 3.9 | 3.4 | 45.8 | 21.8 | 11.4 | 3.1 | 1.9 | 1.2 |
| 100 | 0 | 3.9 | 3.4 | 47.1 | 21.7 | 11.4 | 3.0 | 1.9 | 1.2 |

table shows the log-likelihood values $\chi_{\text {h.s. }}^{2}$ and $\chi_{\text {tot }}^{2}$, without and with the imposition of $\alpha_{s}$ constraints, as defined in Eqs. (10) and (11); as well as $\chi^{2}$ per number of data points for HERA-1 DIS [29] and Tevatron Run-1 and Run-2 single-inclusive jet cross sections [26-28,42,43]. In the fit with a floating $\alpha_{s}$, the best-fit $\alpha_{s}\left(M_{Z}\right)$ is also shown. A comparison of the upper and lower halves of the table shows that the relation between $\chi^{2}$ and $m_{\tilde{g}}$ depends on whether $\alpha_{s}\left(M_{Z}\right)$ is fixed or floating.

Fixed $\alpha_{s}\left(M_{Z}\right)$. In a fit with a fixed $\alpha_{s}\left(M_{Z}\right)$, only constraints from the hadronic data, associated with the term $\chi_{\text {h.s. }}^{2}$ (and not with the total $\chi_{\text {tot }}^{2}$ ) play a meaningful role. The upper half of Table II shows $\chi^{2}$ values from a fit with fixed $\alpha_{s}\left(M_{Z}\right)=0.118$. $^{3}$ In this case, the gluino's effect of slowing the evolution of $\alpha_{s}(Q)$ from $Q=M_{Z}$ to $Q=5 \mathrm{GeV}$ runs into strong disagreement with the low- $Q$

[^252]

FIG. 5 (color online). PDFs for various flavors at $Q=$ 100 GeV , for $m_{\tilde{g}}=50 \mathrm{GeV}$.
constraint; $\chi_{\text {tot }}^{2}$ grows quickly as $m_{\tilde{g}}$ decreases, corresponding to a difference of many standard deviations between the measured and predicted $\alpha_{s}$ values at $Q=5 \mathrm{GeV}$. More importantly, the hadronic data by themselves disfavor very light gluinos, with $m_{\tilde{g}}=25 \mathrm{GeV}$ or less excluded according to the criterion $\Delta \chi^{2} \equiv \chi_{\text {SUSY }}^{2}\left(m_{\tilde{g}}\right)-\chi_{\text {CT10 }}^{2}<100$ applied to $\chi_{\text {h.s. }}^{2}$.

Floating $\alpha_{s}\left(M_{Z}\right)$. The values in the lower half of Table II are for SM+SUSY fits with a variable $\alpha_{s}\left(M_{Z}\right)$. In this case, the constraints from both the hadronic scattering and direct measurements of $\alpha_{s}\left(M_{Z}\right)$ are relevant. The most meaningful log-likelihood term is $\chi_{\text {tot }}^{2}=\chi_{\text {h.s. }}^{2}+\chi_{\alpha_{s}}^{2}$. If $\alpha_{s}\left(M_{Z}\right)$ varies, the hadronic scattering data on their own, including the HERA-1 and Tevatron jet data sets, are compatible with practically any gluino mass. The contribution to $\chi^{2}$ from the hadron scattering experiments, $\chi_{\text {h.s. }}^{2}$, stays approximately the same as in the SM case, or improves slightly, as gluinos with masses of 10,20 , and 50 GeV are introduced.

This agreement with the hadronic scattering data, hardly affected by the gluino mass, results from compensation between modifications in the shape of the gluon PDF and an increase in the preferred $\alpha_{s}\left(M_{Z}\right)$, which grows from 0.118 in the SM case to 0.132 for $m_{\tilde{g}}=10 \mathrm{GeV}$. In contrast, the total likelihood function for the fit to the hadronic scattering data and $\alpha_{s}$ values, introduced as $\chi_{\text {tot }}^{2}$ in Eq. (10), varies considerably as a function of the gluino mass. Our assumed high- $Q$ constraint of $\alpha_{s}\left(M_{Z}\right)=0.123 \pm 0.004$ is slightly higher than $\alpha_{s}\left(M_{Z}\right)=0.118$ obtained by the SM evolution from $\alpha_{s}(Q=5 \mathrm{GeV})=0.213 \pm 0.002$ in Eq. (2). This enhanced value of $\alpha_{s}\left(M_{Z}\right)$ would favor a slower QCD evolution above the gluino mass threshold at about 50 GeV , cf. Figure 2. Consequently, $\chi_{\text {tot }}^{2}$ is smaller at $m_{\tilde{g}}=50 \mathrm{GeV}$ than in the SM case, with the difference dependent on the choice of the high- $Q$ value of $\alpha_{s}\left(M_{Z}\right)$. Specifically, we observe that $\chi_{\text {SUSY }}^{2}\left(m_{\tilde{g}}\right)-\chi_{\mathrm{CT} 10}^{2}$ can be as small as -50 , if we take $\alpha_{s}\left(M_{Z}\right)=0.123 \pm 0.004$, but this difference decreases if a smaller $\alpha_{s}\left(M_{Z}\right)$ is used for the high $-Q$ constraint. For lower gluino masses of 10 or $20 \mathrm{GeV}, \alpha_{s}\left(M_{Z}\right)$ increases and eventually is incompatible with the direct constraints.

## A. $\Delta \boldsymbol{\chi}^{\mathbf{2}}$ as a function of gluino mass

The behavior of $\Delta \chi^{2}$ in the whole range of gluino masses is illustrated by Fig. 6 for a fixed $\alpha_{s}\left(M_{Z}\right)=$ 0.118 , and by Fig. 7 for a floating $\alpha_{s}\left(M_{Z}\right)$. The quantitative likelihood of a given mass $m_{\tilde{g}}$ is specified by $\Delta \chi^{2}=$ $\chi^{2}\left(m_{\tilde{g}}\right)-\chi_{\mathrm{CT} 10}^{2}$, the difference from the $\chi^{2}$ value obtained in the CT10 SM fit. Values of $\Delta \chi^{2}$ in excess of 100 units disfavor an assumed $m_{\tilde{g}}$ at about $90 \%$ C.L. (Refs. [23,39]), while a negative $\Delta \chi^{2}$ indicates a preference for this $m_{\tilde{g}}$. Variations in $\Delta \chi^{2}$ with a magnitude below 100 units can result from a variety of sources and are generally viewed as not significant enough to warrant strong conclusions.

In Fig. 6, two curves are shown for $\Delta \chi_{\text {h.s. }}^{2}$, the difference between the log-likelihoods in the fits performed in the

TABLE II. $\chi^{2}$ values in the global analyses with a floating and fixed $\alpha_{s}\left(M_{Z}\right)$, for various gluino mass values.

|  | SUSY analysis with a fixed $\alpha_{s}\left(M_{Z}\right)=0.118$ |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $m_{\tilde{g}}[\mathrm{GeV}]$ | $\chi_{\text {h.s. }}^{2}$ | $\chi_{\text {tot }}^{2}$ | $\chi^{2} /$ npt: HERA-1 | $\chi^{2} /$ npt: jet prod. | $\alpha_{s}\left(M_{Z}\right)$ |
| 10 | 3154 | 12550 | 1.31 | 1.24 | 0.118 |
| 20 | 3030 | 7882 | 1.24 | 1.19 | 0.118 |
| 50 | 2923 | 3788 | 1.18 | 1.10 | 0.118 |
| $\infty$ | 2918 | 3004 | 1.16 | 1.09 | 0.118 |
|  | SUSY analysis with a floating $\alpha_{s}\left(M_{Z}\right)$ |  |  |  |  |
| $m_{\tilde{g}}[\mathrm{GeV}]$ | $\chi_{\text {h.s. }}^{2}$ | $\chi_{\text {tot }}^{2}$ | $\chi^{2} /$ npt: HERA-1 | $\chi^{2} /$ npt: jet prod. | $\alpha_{s}\left(M_{Z}\right)$ |
| 10 | 2892 | 3124 | 1.14 | 1.06 | 0.132 |
| 20 | 2897 | 2958 | 1.15 | 1.06 | 0.127 |
| 50 | 2896 | 2901 | 1.15 | 1.03 | 0.121 |
| $\infty$ | 2918 | 2960 | 1.16 | 1.09 | 0.118 |



FIG. 6 (color online). Values of $\Delta \chi_{\text {h.s. }}^{2}$ vs $m_{\tilde{g}}$ are shown for a fixed value of $\alpha_{s}\left(M_{Z}\right)=0.118$ for the 2004 study (blue dashed line) and our new one (red solid line).

SM+SUSY and SM scenarios for $\alpha_{s}\left(M_{Z}\right)=0.118$. Here $\Delta \chi_{\mathrm{h} . \mathrm{s} .}^{2}$ is computed from the hadronic scattering contribution only, $\chi_{\text {h.s. }}^{2}$. The blue (dashed) curve represents the 2004 analysis [23]. The red (solid) curve is obtained in the present study, resulting in a tighter lower bound on $m_{\tilde{g}}$. The left branch of the 2010 curve intercepts the $\Delta \chi_{\text {h.s. }}^{2}=$ 100 line at $m_{\tilde{g}} \approx 25 \mathrm{GeV}$. The 2004 curve allows for 15 GeV gluinos and has a broader valley with respect to the 2010 one. This figure shows the improvements in the constraints from the present study, reflecting the inclusion of the latest precise data and technical advances in the the CTEQ analysis since the 2004 publication, including treatment of correlated systematic uncertainties and normalization uncertainties.

Figure 7 illustrates the fits with a variable $\alpha_{s}\left(M_{Z}\right)$. Two curves are shown for $\Delta \chi_{\mathrm{tot}}^{2}$, the difference between the loglikelihoods in the fits performed in the SM+SUSY and SM


FIG. 7 (color online). Values of $\Delta \chi_{\text {tot }}^{2}$ vs $m_{\tilde{g}}$ are shown for varying values of $\alpha_{s}\left(M_{Z}\right)$ for the 2004 study (blue dashed) and our new one (red solid).
scenarios in 2004 (blue dashed line) and 2010 (red solid line). Best-fit values of $\alpha_{s}\left(M_{Z}\right)$ for some gluino masses are indicated by numerical labels near each curve. In this figure, $\Delta \chi_{\mathrm{tot}}^{2}$ is computed from the total function $\chi_{\mathrm{tot}}^{2}$. It includes the direct constraints on $\alpha_{s}(Q)$ in the current study and does not include the $\alpha_{s}$ constraint in the 2004 fit.

The figure emphasizes our earlier observation that the direct $\alpha_{s}$ constraints improve the constraining power of the global analysis. At $m_{\tilde{g}} \rightarrow \infty$, the fit converges to the pure QCD value and $\alpha_{s}\left(M_{Z}\right) \approx 0.119$. According to the $\Delta \chi^{2} \leq$ 100 test, gluinos lighter than 15 GeV are disfavored for all $\alpha_{s}\left(M_{Z}\right)$. Gluinos in the mass range 15 to 50 GeV are allowed if $\alpha_{s}\left(M_{Z}\right)$ takes a value in the range 0.121 to 0.131 . Gluinos heavier than 50 GeV are allowed for practically any $\alpha_{s}\left(M_{Z}\right)$ value. By contrast, the 2004 curve exhibits only a shallow minimum around 5 to 6 GeV , and it is relatively flat as compared to the 2010 curve. The 2004 curve does not establish pronounced lower bounds on $m_{\tilde{g}}$, for a free $\alpha_{s}\left(M_{Z}\right)$.

The 2010 curve in Fig. 7 exhibits an intriguing minimum for a gluino of about 50 GeV , corresponding to $\alpha_{s}\left(M_{Z}\right)$ of 0.121 . Other that noting it, we choose not to base conclusions on this minimum for two reasons. First, from the point of view of the fit itself, given its initial inputs, we adhere to statement that only values of $\left|\Delta \chi^{2}\right|$ in excess of 100 units are considered significant. Second, the depth of this minimum is a reflection of the value of the input constraint $\alpha_{s}\left(M_{Z}\right)=0.123 \pm 0.004$. The dip grows deeper (becomes more shallow) if a larger (smaller) value of the direct constraint is taken at $M_{Z}$. For example, gluinos with mass 50 GeV would be disfavored if the direct constraint $\alpha_{s}\left(M_{Z}\right)<0.118$ were taken, compatible with some existing analyses of LEP data in pure QCD [21,22]. Stronger conclusions on $m_{\tilde{g}}$ await an independent reduction in the uncertainties on $\alpha_{s}\left(M_{Z}\right)$.

## B. Comparison with Tevatron jet cross sections

Table II indicates that the hadronic scattering data, including the combined HERA-1 and Tevatron jet cross sections, may still allow contributions from fairly light gluinos. This observation is somewhat counterintuitive with regard to the precise Tevatron jet cross sections, which could be expected to be sensitive to non-SM contributions in the strong interaction sector. SUSY degrees of freedom introduce new subprocesses in the jet cross sections, such as $g g \rightarrow \tilde{g} \tilde{g}$ and $q \bar{q} \rightarrow \tilde{g} \tilde{g}$. The change in $\alpha_{s}(Q)$ and the alteration of the gluon and quark PDFs also influence the jet rate. However, jet cross section measurements are affected by systematic effects that dominate over statistical uncertainties, notably by the uncertainty on jet energy scale and jet energy resolution. Correlated systematic shifts in the Tevatron jet data must be taken into account when comparisons are made to theory predictions [44]. In our study, systematic uncertainties in the jet data limit the strength of our conclusions.

These observations are illustrated by plots of the CDF Run-2 and D0 Run-2 data vs theory in Figs. 8 and 9. Our results are computed with a floating $\alpha_{s}$. As reference values, we use SM cross sections computed with the CT10 PDFs. Differences from the SM cross section are presented as

$$
\begin{equation*}
\left(\sigma_{i}-\sigma_{\mathrm{CT} 10}\right) / \sigma_{\mathrm{CT} 10} \tag{15}
\end{equation*}
$$

where $\sigma_{i}$ are the SM+SUSY cross sections computed for gluino masses of 10,20 , and 50 GeV . The values of the jet transverse momentum $p_{T}$ are displayed along the horizontal axis. Two bins in the rapidity variable $y$ are shown for each experiment; the behavior in the rest of the bins is similar.

The lower (red) error bars represent the unshifted data. The upper (blue) error bars show the data that are shifted by their systematic uncertainty so as to maximize the agreement with theory for $m_{\tilde{g}}=10 \mathrm{GeV}$. Without the correlated shifts, the data would disfavor the light gluinos with a mass of 10 GeV . The perspective changes significantly if systematic shifts are allowed: the line representing

CDF Run-2 jet production, $\sqrt{ } \mathrm{s}=1.96 \mathrm{TeV}$


FIG. 8 (color online). Comparison of theoretical predictions for single-inclusive jet cross sections with data from CDF Run-2 for two bins in jet rapidity $y$.


FIG. 9 (color online). Same as Fig. 8, for two bins in jet rapidity $y$ in the D0 Run- 2 jet cross section measurement.
$m_{\tilde{g}}=10 \mathrm{GeV}$ now lies completely inside the error bars. Similarly, if $m_{\tilde{g}}$ is equal to 20 or 50 GeV , the effective shifts of the data change to achieve acceptable agreement with the theory curve for this mass. ${ }^{4}$

The systematic uncertainties make it difficult to disfavor the light gluinos solely on the basis of the Tevatron Run-2 jet data. The figures show that the gluino contributions affect the whole $p_{T}$ range, as a result of the momentum sum rule and other connections between the PDFs of different flavors and at different $(x, Q)$ values. Modifications in the jet cross sections due to "new physics" associated with the gluinos cannot be isolated to a specific $p_{T}$ interval, contrary to the assumptions made in some experimental studies of jet cross sections [30].

## VI. CROSS SECTIONS AT THE LHC

The possible existence of color-octet fermions with masses in the range 30 to 100 GeV , allowed by hadronic

[^253]data according to our analysis, raises the prospects for their detection in the extended range of transverse momenta at the LHC. As explained in early sections of this paper, these new fermions modify QCD inputs, primarily the QCD coupling $\alpha_{s}\left(M_{Z}\right)$ and the gluon and sea-quark PDFs. Precise studies of cross sections at LHC energies thus have the potential to reveal differences from pure SM QCD, such as the presence of color-octet fermions, provided the LHC measurements are supplemented by a robust program to reduce uncertainties in $\alpha_{s}, \mathrm{PDFs}$, and other SM parameters, which may otherwise reduce sensitivity of the LHC observables to the gluino contributions.

LHC 7 TeV . Fit with a fixed $\alpha_{s}\left(\mathrm{M}_{\mathrm{Z}}\right)=0.118$


LHC 7 TeV . Fit with a fixed $\alpha_{s}\left(\mathrm{M}_{\mathrm{Z}}\right)=0.118$


FIG. 10 (color online). Ratios of single-inclusive jet cross sections at $\sqrt{s}=7 \mathrm{TeV}$, obtained from the central PDF set of CT10, CT10.00, and the SM+SUSY PDFs for gluino masses $m_{\tilde{g}}=20 \mathrm{GeV}$ (dashed line) and 50 GeV (dot-dashed line). The asymmetric PDF uncertainty of the CT10 set is also shown as a filled band. The SM+SUSY PDFs are obtained under the assumption of $\alpha_{s}\left(M_{Z}\right)=0.118$ for both sets.

Compare, for example, single-inclusive jet cross sections at the LHC energies $\sqrt{s}=7$ and $\sqrt{s}=14 \mathrm{TeV}$, computed at NLO with the Ellis-Kunszt-Soper code named EKS $[45,46]$ in the pure SM case and in the presence of light gluinos. The CT10 asymmetric PDF error bands on the cross sections, normalized to the predictions based on the central CT10.00 PDF set, are also shown in Figs. 10-13 as a function of the jet's transverse momentum $p_{T}$, in several bins of the jet rapidity $y$. Ratios of the expectations based on the SM+SUSY PDFs for $m_{\tilde{g}}=20$ and 50 GeV to their counterparts based on the CT10.00 set are shown as the dashed and dot-dashed lines, respectively.

In Figs. 10 and 11, these ratios are computed with $\alpha_{s}\left(M_{Z}\right)=0.118$ assumed in all PDFs and cross sections. In this case, the SM+SUSY curves lie outside the respective CT10 PDF uncertainty bands for some $p_{T}$, suggesting that the SM and SM+SUSY scenarios can be distinguished, if sufficient experimental accuracy is achieved. On the other


LHC 14 TeV . Fit with a fixed $\alpha_{\mathrm{s}}\left(\mathrm{M}_{\mathrm{Z}}\right)=0.118$


FIG. 11 (color online). Same as Fig. 10 , for $\sqrt{s}=14 \mathrm{TeV}$.
hand, if $\alpha_{s}\left(M_{Z}\right)$ takes the values of 0.126 and 0.121 that are preferred in the SM+SUSY fits with $m_{\tilde{g}}=20$ and 50 GeV , respectively, then the $\mathrm{SM}+\mathrm{SUSY}$ curves lie within the CT10 PDF error bands, as shown in Figs. 12 and 13. In this case, discrimination of the SM and the SM+SUSY cases is more challenging, as reduction of the experimental uncertainty below the current PDF uncertainty would be necessary.

For the inclusive jet cross sections to provide a good discrimination between the SM and SM+SUSY scenarios, the uncertainties on both $\alpha_{s}$ and PDFs must be reduced below the current values. NNLO contributions to SM processes and NLO gluino contributions must also be implemented in both the PDFs and jet cross sections.

A different approach to detecting the presence of new colored states could be based on the expectation that QCD


FIG. 12 (color online). Same as Fig. 10, but with $\alpha_{s}\left(M_{Z}\right)=$ 0.126 in the SM+SUSY calculation with $m_{\tilde{g}}=20 \mathrm{GeV}$, and $\alpha_{s}\left(M_{Z}\right)=0.121$ in the SM+SUSY calculation with $m_{\tilde{g}}=$ 50 GeV .

LHC 14 TeV . Fit with a floating $\alpha_{\mathrm{s}}\left(\mathrm{M}_{\mathrm{Z}}\right)$


FIG. 13 (color online). Same as Fig. 12, for $\sqrt{s}=14 \mathrm{TeV}$.
radiation off a heavy colored object differs from that from massless partons that dominate the inclusive cross sections. It may be possible to identify jets containing gluinos by studying distributions in the jet mass or other jet shapes. The distribution in the jet mass produced by conventional QCD radiation decreases smoothly as the jet mass increases. Decays of gluinos would result in jets whose mass distributions peak at $m_{\tilde{g}}$, and gluino jet contributions could be identifiable above the continuous SM background in the distributions in the jet mass or related observables, using methods being developed [47-50].

## VII. SUMMARY AND DISCUSSION

In this paper, we explore modifications in QCD scattering cross sections introduced by color-octet Majorana fermions in supersymmetry (gluinos) and other popular
extensions of the standard model. Their influence must be included in the evolution of the strong coupling strength and the parton distribution functions, especially if these fermions have mass below 100 GeV (possible in the absence of model-specific assumptions). In addition to modifying the evolution of $\alpha_{s}(Q)$ and the PDFs of the SM quarks and gluons, a relatively light gluino also introduces new production channels such as $g g \rightarrow \tilde{g} \tilde{g}$ in the inclusive jet production case. In this context, hadronic scattering data included in global PDF analyses can provide modelindependent constraints on the color-octet particles.

We examine the values of $\chi^{2}$ obtained from our global fits as a function of the gluino mass $m_{\tilde{g}}$. By analyzing a combination of the latest HERA and Tevatron data on hadronic scattering, and world measurements of the QCD coupling at $Q<10 \mathrm{GeV}$ and $Q=M_{Z}$, we conclude that gluinos must be heavier than 25 GeV at $90 \%$ C.L., if $\alpha_{s}\left(M_{Z}\right)=0.118$, and heavier than 15 GeV if $\alpha_{s}\left(M_{Z}\right)$ is arbitrary. These constraints supersede the 2004 study based on the CTEQ6 data set, in which we found a lower limit on the gluino mass of $m_{\tilde{g}}>12 \mathrm{GeV}$ for $\alpha_{s}\left(M_{Z}\right)=0.118$, and no limit if $\alpha_{s}\left(M_{Z}\right)$ is arbitrary [23]. These new bounds are comparable to the gluino mass bounds $m_{\tilde{g}}>26.9$ and 51 GeV obtained from the analysis of event shapes in $e^{+} e^{-}$hadroproduction at LEP $[16,17]$. Our constraints on $m_{\tilde{g}}$ are obtained from the analysis of inclusive QCD observables and are not affected by theoretical uncertainties of the kind that arise in the determination of $\alpha_{s}\left(M_{Z}\right)$ from the LEP data [18-22] and LEP event shapes.

The changes in $\alpha_{s}\left(M_{Z}\right)$ and in the PDFs of standard model partons must be taken into consideration when QCD tests are made with LHC data. The high energy of the LHC and the extended range in jet transverse momentum offers hope that BSM deviations from pure QCD will show up in inclusive jet cross sections. As discussed in our comparisons with Tevatron jet data, it will be critical to control experimental uncertainties on the jet energy scale and jet energy resolution. Gluino contributions and adjustments in the SM parameters tend to offset one another. The power of precise measurements of the LHC single-inclusive jet cross sections will be enhanced provided that $\alpha_{s}\left(M_{Z}\right)$ and the PDFs for gluons and quarks are constrained more tightly than now by measurements in other channels.

For the purpose of studying jet properties in detail, we provide routines to interface with the SM+gluino PDFs. These are linked from the CTEQ webpage at cteq.org. We also note that the MADGRAPH/MADEVENT programs [51] provide a mechanism to incorporate SUSY PDFs in the initial state; information for using this interface is also provided on the webpage.

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## APPENDIX A: MODIFICATION OF THE STRONG COUPLING

The running of $\alpha_{s}(Q)$ must be matched to the individual PDF set with the appropriate mass thresholds. The expansion of the evolution equation for $\alpha_{s}(Q)$,

$$
\begin{align*}
Q \frac{\partial}{\partial Q} \alpha_{s}(Q) & =-\frac{\alpha_{s}^{2}}{2 \pi} \sum_{n=0}^{\infty} \beta_{n}\left(\frac{\alpha_{s}}{4 \pi}\right)^{n} \\
& =-\left[\beta_{0} \frac{\alpha_{s}^{2}}{2 \pi}+\beta_{1} \frac{\alpha_{s}^{3}}{2^{3} \pi^{2}}+\ldots\right] \tag{A1}
\end{align*}
$$

can be solved perturbatively. It takes the form [52]

$$
\begin{align*}
\alpha_{s}(Q)= & \frac{4 \pi}{\beta_{0} \ln \left(\frac{Q^{2}}{\Lambda^{2}}\right)}\left[1-\frac{\beta_{1}}{\beta_{0}^{2}} \frac{\ln \left[\ln \left(Q^{2} / \Lambda^{2}\right)\right]}{\ln \left(Q^{2} / \Lambda^{2}\right)}\right. \\
& \left.+\frac{\beta_{1}^{2}}{\beta_{0}^{4} \ln ^{2}\left(Q^{2} / \Lambda^{2}\right)}+\cdots\right] . \tag{A2}
\end{align*}
$$

The beta functions, $\beta_{0}$ and $\beta_{1}$ depend on the number of active fermions and bosons. When supersymmetric particles are included [53], the first two coefficients in Eq. (A2) are

$$
\beta_{0}=11-\frac{2}{3} n_{f}-2 n_{\tilde{g}}-\frac{1}{6} n_{\tilde{f}},
$$

and

$$
\begin{equation*}
\beta_{1}=102-\frac{38}{3} n_{f}-48 n_{\tilde{g}}-\frac{11}{3} n_{\tilde{f}}+\frac{13}{3} n_{\tilde{g}} n_{\tilde{f}}, \tag{A3}
\end{equation*}
$$

where $n_{f}$ is the number of quark flavors, $n_{\tilde{g}}$ is the number of gluinos, and $n_{\tilde{f}}$ is the number of squark flavors. As the evolution proceeds across mass thresholds, these numbers and, consequently $\alpha_{s}$, must be adjusted.

## APPENDIX B: GLUINO CONTRIBUTIONS TO THE SINGLE-INCLUSIVE JET CROSS SECTION

The leading-order cross section for inclusive (di)jet production, $H_{1} H_{2} \rightarrow j\left(p_{3}\right) j\left(p_{4}\right) X$, expressed in terms of the transverse momentum $p_{T}$ and rapidities $y_{3}, y_{4}$ of the jets, is

$$
\begin{align*}
\frac{d \sigma}{d p_{T} d y_{3} d y_{4}}= & \frac{2 \pi \alpha_{s}^{2} p_{T}}{\hat{s}^{2}} \sum_{i, j} x_{1} x_{2} f_{H_{1} \rightarrow i}\left(x_{1}, \mu_{F}^{2}\right) \\
& \times f_{H_{2} \rightarrow j}\left(x_{2}, \mu_{F}^{2}\right) \sum_{\text {spin }}\left|\mathcal{M}_{p_{1} p_{2} \rightarrow p_{3} p_{4}}\right|^{2} \tag{B1}
\end{align*}
$$

where $x_{1}=m_{T} / \sqrt{s}\left(e^{y_{3}}+e^{y_{4}}\right)$, and $x_{2}=m_{T} / \sqrt{s}\left(e^{-y_{3}}+\right.$ $\left.e^{-y_{4}}\right)$ are the parton momentum fractions, $m_{T}^{2}=p_{T}^{2}+m_{\tilde{g}}^{2}$ is the gluino's transverse mass, and $\sqrt{s}$ is the collider center-of-mass energy. In our analysis, scattering amplitudes for subprocesses with gluino pair production, $g g \rightarrow$ $\tilde{g} \tilde{g}$ and $q \bar{q} \longrightarrow \tilde{g} \tilde{g}$, are included with full dependence on gluino mass $m_{\tilde{g}}$. Scattering amplitudes for the other LO subprocesses (with at least one initial-state gluino) are evaluated in the $m_{\tilde{g}}=0$ approximation, in accord with the S-ACOT factorization scheme [34,35].

SUSY contributions with full mass dependence can be found in the literature (e.g., in $[37,54]$ ), but they are presented here in a consistent notation for completeness. In terms of the usual parton-level Mandelstam variables, $\hat{s}=\left(p_{1}+p_{2}\right)^{2}, \hat{t}=\left(p_{1}-p_{3}\right)^{2}$, and $\hat{u}=\left(p_{1}-p_{4}\right)^{2}$, the square of the amplitude for $q \bar{q} \rightarrow \tilde{g} \tilde{g}$ is

$$
\begin{align*}
\left|\mathcal{M}_{q \bar{q} \rightarrow \tilde{g} \tilde{g}}\right|^{2}= & \frac{8}{9}\left[\frac{\hat{s} m_{\tilde{g}}^{2}}{3\left(m_{\tilde{q}}^{2}-\hat{t}\right)\left(m_{\tilde{q}}^{2}-\hat{u}\right)}+\frac{4\left(m_{\tilde{g}}^{2}-\hat{t}\right)^{2}}{3\left(m_{\tilde{q}}^{2}-\hat{t}\right)^{2}}\right. \\
& -\frac{3\left(\hat{s} m_{\tilde{g}}^{2}+\left(m_{\tilde{g}}^{2}-\hat{t}\right)^{2}\right)}{\hat{s}\left(m_{\tilde{q}}^{2}-\hat{t}\right)}+\frac{4\left(m_{\tilde{g}}^{2}-\hat{u}\right)^{2}}{3\left(m_{\tilde{q}}^{2}-\hat{u}\right)^{2}} \\
& -\frac{3\left(\hat{s} m_{\tilde{g}}^{2}+\left(m_{\tilde{g}}^{2}-\hat{u}\right)^{2}\right)}{\hat{s}\left(m_{\tilde{q}}^{2}-\hat{u}\right)} \\
& \left.+\frac{3\left(2 \hat{s} m_{\tilde{g}}^{2}+\left(m_{\tilde{g}}^{2}-\hat{t}\right)^{2}+\left(m_{\tilde{g}}^{2}-\hat{u}\right)^{2}\right)}{\hat{s}^{2}}\right] . \tag{B2}
\end{align*}
$$

Here $m_{\tilde{q}}$ is the mass of the squark, and the prefactor $8 / 9$ is a color factor. We report the expression with all the fermion mass dependence, but in our computations we have taken the limit $m_{\tilde{q}} \rightarrow \infty$.

The square of the amplitude for $g g \rightarrow \tilde{g} \tilde{g}$ is


FIG. 14 (color online). Parton-parton luminosity $\tau d \mathcal{L}_{i j}(\tau, Q) / d \tau$ vs $\sqrt{\tau}$ for $m_{\tilde{g}}=50 \mathrm{GeV}$ at $Q=100$ and 300 GeV .

$$
\begin{align*}
\left|\mathcal{M}_{g g \rightarrow \tilde{g} \tilde{g}}\right|^{2}= & -\frac{9 m_{\tilde{g}}^{6}}{4 \hat{s}^{2}\left(\hat{t}-m_{\tilde{g}}^{2}\right)}-\frac{9 m_{\tilde{g}}^{6}}{4 \hat{s}^{2}\left(\hat{u}-m_{\tilde{g}}^{2}\right)}+\frac{27 \hat{u} m_{\tilde{g}}^{4}}{4 \hat{s}^{2}\left(\hat{t}-m_{\tilde{g}}^{2}\right)}-\frac{45 m_{\tilde{g}}^{4}}{2 \hat{s}\left(\hat{t}-m_{\tilde{g}}^{2}\right)}+\frac{27 \hat{t} m_{\tilde{g}}^{4}}{4 \hat{s}^{2}\left(\hat{u}-m_{\tilde{g}}^{2}\right)}-\frac{45 m_{\tilde{g}}^{4}}{2 \hat{s}\left(\hat{u}-m_{\tilde{g}}^{2}\right)} \\
& +\frac{27 m_{\tilde{g}}^{4}}{\left(\hat{t}-m_{\tilde{g}}^{2}\right)\left(\hat{u}-m_{\tilde{g}}^{2}\right)}+\frac{9 m_{\tilde{g}}^{4}}{\hat{s}^{2}}-\frac{81 m_{\tilde{g}}^{4}}{\left(\hat{t}-m_{\tilde{g}}^{2}\right)^{2}}-\frac{81 m_{\tilde{g}}^{4}}{\left(\hat{u}-m_{\tilde{g}}^{2}\right)^{2}}-\frac{27 \hat{u}^{2} m_{\tilde{g}}^{2}}{4 \hat{s}^{2}\left(\hat{t}-m_{\tilde{g}}^{2}\right)}-\frac{9 \hat{t} m_{\tilde{g}}^{2}}{\hat{s}^{2}}+\frac{45 \hat{u} m_{\tilde{g}}^{2}}{2 \hat{s}\left(\hat{t}-m_{\tilde{g}}^{2}\right)}-\frac{9 \hat{u} m_{\tilde{g}}^{2}}{\hat{s}^{2}} \\
& +\frac{9 m_{\tilde{g}}^{2}}{\hat{s}}-\frac{27 \hat{t}^{2} m_{\tilde{g}}^{2}}{4 \hat{s}^{2}\left(\hat{u}-m_{\tilde{g}}^{2}\right)}+\frac{45 \hat{t} m_{\tilde{g}}^{2}}{2 \hat{s}\left(\hat{u}-m_{\tilde{g}}^{2}\right)}+\frac{9 \hat{t}^{2}}{4 \hat{s}^{2}}+\frac{9 \hat{u}^{2}}{4 \hat{s}^{2}}+\frac{9 \hat{t} \hat{u}}{2 \hat{s}^{2}}+\frac{9 \hat{u}^{3}}{4 \hat{s}^{2}\left(\hat{t}-m_{\tilde{g}}^{2}\right)}+\frac{9 \hat{t}^{3}}{4 \hat{s}^{2}\left(\hat{u}-m_{\tilde{g})}^{2}\right.} . \tag{B3}
\end{align*}
$$

## APPENDIX C: PARTON LUMINOSITIES

Parton-parton luminosity functions portray the relative size of various partonic contributions. The parton luminosity is defined as a convolution integral of the PDFs $f_{i}(\xi, Q)$ for two incoming partons $(i, j=\tilde{g}, g, u, d, s, \ldots)$ :

$$
\frac{d \mathcal{L}_{i j}(\tau, Q)}{d \tau}=f_{i} \otimes f_{j}=\int_{\tau}^{1} \frac{d \xi}{\xi} f_{i}(\xi, Q) f_{j}\left(\frac{\tau}{\xi}, Q\right)
$$

where $\tau=\hat{s} / s$. Here $\hat{s}$ is the square of the center-of-mass energy in the incident parton-parton system. In terms of this luminosity, the production cross section for a specific reaction is

$$
\begin{equation*}
\sigma(s)=\sum_{i, j} \int_{\tau_{0}}^{1} d \tau \hat{\sigma}_{i j}(\tau) \frac{d \mathcal{L}_{i j}(\tau, Q)}{d \tau} \tag{C1}
\end{equation*}
$$

The sum is over the initial-state parton flavors $i$ and $j$, and $\hat{\sigma}_{i j}(\tau)$ is the partonic cross section for the subprocess initiated by partons $i, j$.

The luminosities for some flavor combinations are shown in Fig. 14 for $m_{\tilde{g}}=50 \mathrm{GeV}$. At $Q=100 \mathrm{GeV}$ all gluino luminosities are smaller than the SM luminosities,
but they grow in magnitude as $Q$ increases. The gluongluino luminosity is roughly the same as the gluon-bottom quark luminosity, as would be expected from the momentum fractions presented in Table I. At $Q=300 \mathrm{GeV}$ the $\tilde{g} \otimes g$ contribution is comparable to that of the ordinary quarks. The $\tilde{g} \otimes g$ combination is smaller than $s \otimes g$ throughout the $x$ range for $Q=100 \mathrm{GeV}$. At $Q=$ 300 GeV , the evolution of the gluino is enhanced, and $\tilde{g} \otimes g$ exceeds various SM pairings for $x>0.1$.
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# CT10 parton distributions and other developments in the global QCD analysis 

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#### Abstract

We summarize several projects carried out by the CTEQ global analysis of parton distribution functions (PDFs) of the proton during 2010. We discuss a recently released CT10 family of PDFs with a fixed and variable QCD coupling strength; implementation of combined HERA and Tevatron lepton asymmetry data sets; theoretical issues associated with the analysis of $W$ charge asymmetry in PDF fits; PDFs for leading-order shower programs; and constraints on new color-octet fermions from the hadronic data.


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## CTEQ PDFs in 2010

Parton distribution functions (PDFs) are essential nonperturbative functions of quantum chromodynamics (QCD). They describe the internal structure of the proton in high-energy scattering at the Fermilab Tevatron collider, CERN Large Hadron Collider, and in other experiments. Modern PDFs continuously evolve to include emerging theoretical developments and latest data from hadronic experiments, and to provide reliable estimates of uncertainties associated with various experimental and theoretical inputs. In this paper, we review the recent progress in the determination of the PDFs by CTEQ collaboration [1, 2, 3, 4], which is one of three groups involved in the global analysis of hadronic data, besides the MSTW [5] and NNPDF [6] groups.

## Implementation of new data sets

Since the release of the previous general-purpose CTEQ6.6 PDF set [7] in 2008, new data sets have been published in every category of processes included in the global QCD analysis: deep inelastic scattering (DIS), vector boson production, and inclusive jet production. These data sets include a combination of DIS cross sections by the H1 and ZEUS collaborations in HERA-1 [8], as well as measurements of $W$ lepton asymmetry $[9,10,11], Z$ rapidity distributions $[12,13]$, and single-inclusive jet cross sections $[14,15]$ by CDF and D $\emptyset$ collaborations at the Tevatron. All these new data are included in our latest global analysis, designated as CT10 [3].

The new analysis produced two families of general-purpose PDF sets, denoted as CT10 and CT10W, which differ in their treatment of the Tevatron $W$ lepton asymmetry data sets affecting the ratio of $d$ and $u$ quark PDFs at $x>0.1$, as discussed below, but are very similar in all other aspects. In addition, we examined the dependence of the PDFs on the QCD coupling $\alpha_{s}\left(M_{Z}\right)$ and provided special CT10AS PDF sets with a varied $\alpha_{s}\left(M_{Z}\right)$ in the range 0.113-0.123 to evaluate the combined PDF- $\alpha_{s}$ uncertainty in practical applications. The CT10 PDFs are obtained at next-toleading order in $\alpha_{s}$, using the general-mass treatment of charm and bottom quark contributions to hadronic observables. To support calculations for heavy-quark production in the fixed-flavornumber factorization scheme, we also provide additional PDF sets CT10(W). 3 F and CT10(W). 4 F , obtained from the best-fit CT10.00 and CT10W PDF sets by QCD evolution with three and four active quark flavors. All the PDF sets discussed in this paper (CT10, CT10W, CT10AS, CT10XF, and CT09MC) are available as a part of the LHAPDF library [16] and from our website [17].

## Constraints from combined DIS data by HERA-1

The CT10/CT10W fits include a combined set of HERA-1 cross sections on neutral-current and charged-current DIS [8], which replaces 11 separate HERA-1 data sets used in CTEQ6.6 and earlier fits. In the combined set, systematic factors that are in common to both experiments were presented as a table of 114 correlated systematic errors, whose effect is shared by each data point in all scattering channels. As a result of the cross calibration of detection parameters between the H1 and ZEUS experiments, the combined data set has a reduced total systematic uncertainty. Consequently, the PDF uncertainties at $x<10^{-3}$, in the region where the HERA data provide tightest constraints on the gluon and heavy-quark PDFs, are also reduced.

The impact of the combined HERA-1 set on the PDFs is illustrated by Fig. 1, showing relative differences between the CT10 PDF set, fitted to the combined HERA-1 data, and a counterpart fit, fitted to the separate HERA-1 data sets. In the left subfigure, comparing the best-fit PDFs in the two fits, one observes reduction in the gluon and charm PDFs at $x<0.05$, accompanied by a few-percent increase in the $u$ and $d$ quark PDFs in the same $x$ region. The strange quark PDF shows a larger suppression (up to $25 \%$ at $x=10^{-5}$ ), which, however, is small compared to the large

Figure 1: Left: ratios of CT10 central PDFs fitted to the combined HERA-1 data set and to the separate HERA-1 data sets, at scale $\mu=2 \mathrm{GeV}$. Right: bands of the PDF uncertainty (relative to the the central PDF set) for the gluon PDF in (red) CT10 with the combined HERA-1 data, (blue) CT10 with the separate HERA data. $g(x), Q=2 \mathrm{GeV}$.



PDF uncertainty associated with this flavor. Fig. 1 (right) shows the asymmetric fractional PDF uncertainty, computed as in [18], and normalized to the best-fit gluon PDF of each fit. The impact of the HERA-1 data on the uncertainties of the gluon and charm PDFs is visible in the small- $x$ region, starting from $x=10^{-3}$ and going down to $x=10^{-5}$, where the error bands contract upon the combination of the HERA data sets. In the large $x$ region, the error bands for the combined and separate HERA data sets are almost coincident.

## Agreement with the HERA data at small and large $x$

The overall agreement of the CT10 fit with the combined HERA-1 data is slightly worse than with the separate HERA-1 data sets, as a consequence of some increase in $\chi^{2} /$ d.o.f. for the neutralcurrent DIS data at $x<0.001$ and $x>0.1$. While the origin of this increase is uncertain, the pattern of point-to-point contributions to $\chi^{2}$ from the data is consistent with random fluctuations that turn out to be larger than normally expected. No systematic discrepancies between the HERA-1 DIS data and theoretical cross sections are observed, suggesting that the NLO QCD theory based on CT10 PDFs is generally consistent with the HERA experiments in the region $Q>2 \mathrm{GeV}$ included in the CT10 fit.

In looking for potential systematic deviations of this kind, we examined the agreement with the data as a function of either $x$ and $Q$, or the "geometric scaling" variable $A_{g s}=Q^{2} x^{0.3}$ proposed by NNPDF authors in Refs. [19, 20]. At $A_{g s} \rightarrow 0$, DGLAP factorization that is required to introduce the PDFs can be invalidated by higher-twist terms or saturation; the question is whether such effects may bias the determination of the PDFs at $A_{g s} \gtrsim 0.1$, in the kinematical region commonly included in the global fits.

Indeed, the NNPDF study finds that the PDFs fitted to the HERA data above some cutoff value $\left(A_{g s}>A_{c u t}\right)$, disagree at the $2 \sigma$ level with the HERA data in the "causally connected" region below the cutoff, $0.5<A_{g s}<A_{c u t}$. The NNPDF analysis is realized in the zero-mass approximation and includes DIS data in the less safe region $\sqrt{2} \mathrm{GeV}<Q<2 \mathrm{GeV}$. We repeated the $A_{\text {cut }}$ fits proposed by NNPDF as closely as possible, in the general-mass factorization scheme, and in the region of $Q>2 \mathrm{GeV}$ where our data are customarily selected to suppress higher-order

Figure 2: Comparison of CDF Run-2 lepton asymmetry data [9] with LO, NLO, and resummed predictions from ResBos [35].

and higher-twist terms. While the outcomes of our $A_{\text {cut }}$ fits bear some similarity to those by NNPDF, the discrepancies between our best-fit NLO predictions and the data below $A_{\text {cut }}$ are less significant than those quoted by NNPDF and are characterized by a large PDF uncertainty. Thus, our fits do not corroborate the existence of stable deviations of the NLO DGLAP factorization from the data, if the lower $Q$ bound is chosen to be above 2 GeV . See further discussion in the appendix of Ref. [3].

## Tevatron Run-2 W lepton asymmetry data

The puzzle of Run-2 W asymmetry. Recently, the Fermilab DØ Collaboration [10, 11] published measurements of $W$ charge asymmetry $A_{\ell}\left(y_{\ell}\right)$ in electron $(\ell=e)$ and muon $(\ell=\mu)$ decay channels, presented as a function of the rapidity of the charged decay lepton. NLO predictions based on CTEQ6.1 and CTEQ6.6 sets disagree with these data at surprisingly large $\chi^{2} / N p t$ of about 5 . The values of $\chi^{2} / N p t$ can be even higher (as high as 20 ) for some other recent (N)NLO PDF sets [11, 22]. Such level of disagreement may appear surprising, given that the Tevatron $W$ asymmetry probes the ratio of $d$ and $u$ quark PDFs [21] in the region $x>0.1$, where they are known quite well from the other experiments.

Sensitivity to the $d / u$ slope. The discrepancy involving $A_{\ell}$ can be understood in part by noticing that the $A_{\ell}$ measurement is very sensitive to the average $x$ derivative (slope) of the ratio of the up and down quark PDFs, $d\left(x, M_{W}\right) / u\left(x, M_{W}\right)$, computed between the typical $x$ values $x_{1,2}=M_{W} e^{ \pm y_{W}} / \sqrt{s}$ accessible at a given boson rapidity $y_{W}[21,23]$. Small variations of the $d / u$ slopes in distinct PDF sets can change the behavior of $A_{\ell}$ by large amounts [24].

Impact of soft gluon resummation. Another factor at play are soft parton emissions with small transverse momenta, which affect the precise $A_{\ell}$ data because of constraints imposed on the transverse momentum $p_{T \ell}$ of the decay charged lepton. The $A_{\ell}$ data require $p_{T \ell}$ to be above 20-25 GeV in order to suppress charged leptons from background processes that do not involve a $W$ boson decay. In addition, the Run- $2 A_{\ell}$ data are organized into bins of $p_{T \ell}$, e.g., $25-35 \mathrm{GeV}$ and $35-45$ GeV in order to better probe the $x$ dependence of $d(x, Q) / u(x, Q)$ [9]. While such binning amplifies the sensitivity of the $A_{\ell}$ data to the PDFs, it also makes it dependent on the shape of the $p_{T \ell}$ distribution near the Jacobian peak at $p_{T \ell} \approx M_{W} / 2 \approx 40 \mathrm{GeV}$ or, equivalently, to the transverse momentum $\left(Q_{T}\right)$ distribution of $W$ bosons at $Q_{T}<20 \mathrm{GeV}$, where large logarithms $\ln \left(Q_{T} / Q\right)$ dominate the cross section. A calculation that evaluates these logarithms to all orders in $\alpha_{s}[25,26$, $27]$, in addition to including the leading NNLO corrections [29, 28], results in somewhat different

Figure 3: Comparison of the CT10W and CTEQ6.6 predictions with the DØ Run-II data for the electron charge asymmetry $A_{e}\left(y_{e}\right)$ for an integrated luminosity of $0.75 \mathrm{fb}^{-1}$ [10]




Figure 4: The $d / u$ ratio for CT10 (left) and CT10W (right) versus that for CTEQ6.6, at scale $\mu=85 \mathrm{GeV}$.


predictions for $A_{\ell}$ than (N)NLO calculations without resummation, like those implemented in the other available codes $[30,32,33,34]$.

In CT10 fits, the QCD radiative contributions to $A_{\ell}\left(y_{\ell}\right)$ are implemented to the next-to-next-to-leading accuracy in $Q_{T}$ logarithms and NLO accuracy in the QCD coupling strength using the program ResBos that realizes the approach of Refs. [25, 26, 27]. The resummed differential distributions for $d \sigma / d Q_{T}$ and $d \sigma / d p_{T \ell}$ both agree well with the data, in contrast to the fixed-order results. We thus expect that the resummed predictions for $A_{\ell}$ implemented in the CT10 fit are more reliable as well.

The magnitude of differences between the NLO and resummed predictions is illustrated by Fig. 2, comparing the CDF Run-2 $A_{\ell}\left(y_{\ell}\right)$ data [9] with LO, NLO, and resummed NNLL-NLO predictions from ResBos. The NLO and resummed curves are clearly distinct in the bin $25<p_{T \ell}<$ 35 GeV , shown in the left panel, and some differences are also seen in the bin $35<p_{T \ell}<45 \mathrm{GeV}$, shown in the right panel. The shape of the NLO prediction in this comparison is not unique and depends on the phase space slicing parameter $Q_{T}^{\text {sep }}$ that defines the size of the lowest $Q_{T}$ bin where the real and virtual NLO singularities are canceled [26]. In the current comparison, $Q_{T}^{s e p}=3 G e V$, but other values of $Q_{T}^{s e p}$ are equally possible and would lead to NLO predictions lying closer to, or further from, the shown resummed curve. Such variations due to $Q_{T}^{s e p}$ or factorization scale indicate that resummation effects are important and should be included in precise fits to $A_{\ell} .{ }^{1}$

Numerical predictions of the CT10W analysis. When included in the CTEQ global analysis, the CDF measurements of $A_{\ell}$ in Tevatron Run-1 [37] and Run-2 [9] agree well with the other data sets constraining the $d / u$ ratio, provided by deep inelastic scattering on proton and

[^254]deuteron targets by the NMC [38] and BCDMS [39, 40] collaborations. However, the most precise Run-2 lepton $A_{\ell}$ data by the $\mathrm{D} \emptyset$ Collaboration $[10,11]$ run into disagreement with the NMC and BCDMS deuteron DIS data, and in addition, exhibit some tension among themselves. Because of these disagreements, two separate fits are produced: CT10, which does not contain the DØ $W$ electron asymmetry sets, and CT10W, in which they are included using weight factors larger than 1 to ensure an acceptable fit. We obtain $\chi^{2} / N p t=91 / 45=2$ in the CT10W fit to the Run- 2 $A_{\ell}$, which is a significant improvement compared to $200 / 45=4.4$ obtained in CT10. Comparison of NNLL-NLO predictions based on CT10W PDFs with the electron charge asymmetry data is presented in Fig. 3.

In the CT10W analysis, the inclusion of the Run- $2 A_{\ell}$ data increases the slope of $d(x) / u(x)$ at $x$ between 0.1 and 0.5 and reduces its uncertainty, as compared to CTEQ6.6 and CT10. This is illustrated by Fig. 4, which shows uncertainty bands for the $d / u$ ratio in CTEQ6.6, CT10, CT10W PDFs vs. the momentum fraction $x$ at scale $Q=85 \mathrm{GeV}$.

Fig. 5 shows the ratios $r_{W Z}=\sigma\left(p p \rightarrow W^{ \pm} X\right) / \sigma\left(p p \rightarrow Z^{0} X\right)$ and $r_{W^{+} W^{-}}=\sigma(p p \rightarrow$ $\left.W^{+} X\right) / \sigma\left(p p \rightarrow W^{-} X\right)$ of the rapidity distributions in $W^{ \pm}$and $Z$ boson production at the LHC, obtained using CTEQ6.6, CT10 and CT10W PDFs and divided by the predictions based on the CTEQ6.6M set. Here, the reduction of the uncertainty bands in the ratio of $W^{+}$to $W^{-}$cross sections predicted based on the CT10W PDFs, as compared to CT10, is again evident.

Comparison with other fits. The MSTW'08 [5] and NNPDF2.0 [36] groups have also explored the impact of the $\mathrm{D} \emptyset$ Run- $2 A_{\ell}$ data. While their conclusions are broadly compatible with ours, the details vary. For example, in the CT10W fit, we find that all three $p_{T \ell}$ bins of the electron $A_{\ell}$ data and the second $p_{T \ell}$ bin of the fit can be combined with the other data sets, despite the remaining disagreement with the deuteron DIS experiments. NNPDF, on the other hand, finds that all bins of the muon $A_{\ell}$ are compatible with the deuteron DIS and all other experiments, but incompatible with the second and third $p_{T \ell}$ bins of the electron $A_{\ell}$. NNPDF compute their NLO $A_{\ell}$ predictions using the DYNNLO code [34], which can deviate from the resummed NNLL + NLO predictions by ResBos used by CTEQ, as discussed above.

The resolution of the Run- $2 A_{\ell}$ puzzle thus seems to require consistent implementation of perturbative QCD calculations both in experimental analyses and PDF fits, including small- $Q_{T}$ resummed contributions, when constraints on the lepton $p_{T \ell}$ are imposed. For greater precision it may be preferable to perform the small- $Q_{T}$ resummation for every component of the angular distribution of the decay lepton [41], in addition to the resummation for two dominant angular components that is currently implemented in ResBos. Resummation of the full dependence on the polar and azimuthal angles $\theta$ and $\phi$ of the lepton in the vector boson rest frame may be important especially in situations in which the experimental coverage is not uniform in all directions, or when there are gaps in the coverage. Normally the angular coverage varies with rapidity, notably at large rapidity, and this variation may well affect the lepton asymmetry, with different consequences in different experiments.

Figure 5: CT10, CT10W, and CTEQ6.6 PDF uncertainty bands for the ratios $\left(d \sigma\left(W^{ \pm}\right) / d y\right) /(d \sigma(Z) / d y)$ (upper two subfigures) and $\left(d \sigma\left(W^{+}\right) / d y\right) /\left(d \sigma\left(W^{-}\right) / d y\right)$ (lower two subfigures), at the LHC energies 7 and 14 TeV .


## CT10 predictions for collider observables

Fig. 6 compares the NLO total cross sections, obtained using CT10 and CT10W PDFs, to those obtained using CTEQ6.6 PDFs, for some selected processes at the Tevatron Run-2 and the LHC at $\sqrt{s}=7 \mathrm{TeV}$. For most of the cross sections, CT10 and CT10W sets provide similar predictions and uncertainties, which are also in good agreement with those from CTEQ6.6 (i.e., well within the PDF uncertainty band). At the LHC, the PDF uncertainties in CT10 and CT10W predictions for some processes are larger than those in the counterpart CTEQ6.6 predictions, reflecting the changes in the framework of the fit discussed in the next paragraph. At the Tevatron, the CT10(W) PDF uncertainties tend to be about the same as those for CTEQ6.6, with a notable exception of $t \bar{t}$ production cross sections, which have a smaller PDF uncertainty with the CT10W set, because of stricter constraints on the up- and down-quark PDFs at the relevant $x$ values.

## New PDF parametrizations; advancements in statistical analysis

The CT10 global analysis implements several new features which were not available in the previous studies. The systematic uncertainty associated with the overall normalization factor in each of the data sets is handled in the same manner that all other systematic error parameters are handled. The best-fit values of the normalizations are found algebraically, and their variations are included in the final estimate of the PDF uncertainties. More flexible parametrizations are assumed for the gluon, $d$-quark, and strange quark PDFs at the initial scale 1.3 GeV , to reduce biases in predictions in kinematical regions where the constraints from the data are weak. Finally, a new statistical procedure is introduced to guarantee the agreement of the fits at $90 \%$ C.L. with all included experiments, for any PDF eigenvector set produced by the error analysis. This is realized by adding an extra contribution to the total $\chi^{2}$, which guarantees the quality of fit to each individual data set and halts the displacement along any eigenvector early, if necessary, to prevent one or more individual data sets from being badly described. The old procedure to enforce the $90 \%$ C.L. agreement with all experiments in the CTEQ6 family of fits, by artificially increasing statistical weights of $\chi^{2}$ contributions from those experiments that may be fitted poorly by some PDF eigenvector sets, is phased out by this more efficient method. As a result of these changes, the CT10/CT10W PDF uncertainty may be smaller or larger than the CTEQ6.6 uncertainty, depending on whether the improved constraints from the data outweigh the increased uncertainty due to the relaxed PDF parametrizations and variations of normalizations during the determination of PDF eigenvector sets.

## Dijet invariant mass distributions

Fig. 7 compares NLO predictions based on CTEQ6.6, CT10, and CT10W PDFs with the data on the dijet invariant mass distribution $d \sigma / d M_{j j}$ reported recently by the $\mathrm{D} \emptyset$ Collaboration [42]. These data are not included in the CT10 fit, but they are sensitive to the same scattering subprocesses, and include the same events, as the single-inclusive jet data constraining the gluon PDF in the CT10 fit. The cross sections are normalized to the theory prediction based on the central CT10 PDF set. The statistical and systematic errors of the D $\varnothing$ data are added in quadrature. The renormalization and factorization scales in the theoretical predictions are set equal to a half of the average $p_{T}$ of the jets, $\left\langle p_{T}\right\rangle / 2$, consistent with the scale used in the single-jet cross sections when determining the gluon PDFs. With this choice of the scale, all three PDF sets agree with most of the data points within the PDF uncertainty. There appears to be a systematic excess of theory over the data, but its magnitude strongly depends on the assumed factorization scale. For example, it can be much worse if a different scale is taken, such as $\mu=\left\langle p_{T}\right\rangle$ assumed in Fig.

Figure 6: Ratios of NLO total cross sections obtained using CT10 and CT10W to those using CTEQ6.6M PDFs, in various scattering processes at the Tevatron Run-II and LHC.





Figure 7: Comparison of DØ Run-II data for dijet invariant mass distributions [42] with NLO theoretical predictions and their PDF uncertainties for CTEQ6.6 (black), CT10 (red) and CT10W (blue) PDFs. The cross sections are normalized to theoretical predictions based on the best-fit CT10 set, designated as CT10.00.


2 of the D $\emptyset$ paper [42]. We conclude that the CT10 PDFs are reasonably compatible with the $\mathrm{D} \emptyset$ dijet data within the present theoretical uncertainties, although an overall systematic shift, of order of the systematic shifts observed in the CT09 study of the single-inclusive jet distributions [1], would further improve the agreement, once the full correlated systematic errors of the dijet data become available.

## Uncertainty due to $\alpha_{s}$ in CTEQ6.6 and CT10 PDF analyses

Many calculations for collider processes (e.g., production of $t \bar{t}$ pairs and Standard Model Higgs bosons) require to evaluate two leading theoretical uncertainties, due to the choice of the PDF parametrization at the initial scale, and the value of the strong coupling constant $\alpha_{s}\left(M_{Z}\right)$ assumed in the hard cross sections and the PDFs. These uncertainties can be comparable in size, and their interplay, or correlation, may be important. In Ref. [2], we examine the $\alpha_{s}$ dependence of CTEQ6.6 PDFs [7] and show how the PDF- $\alpha_{s}$ correlations are adequately captured by a simple calculation, without resorting to more elaborate methods proposed in other studies [43].

At the beginning of the PDF fit, one decides which data determine the $\alpha_{s}\left(M_{Z}\right)$ value and its uncertainty. CTEQ best-fit PDFs and their parametrization uncertainties are usually determined for a constant value of $\alpha_{s}\left(M_{Z}\right)$ that is close to its latest world-average central value; e.g., $\alpha_{s}\left(M_{Z}\right)=$ $0.118 \pm 0.002$ assumed in Ref. [2]. This input value of $\alpha_{s}\left(M_{Z}\right)$ can be viewed as an additional data point that summarizes world constraints on $\alpha_{s}$, mostly determined by precise experiments that are not included in the global fit (notably, LEP event shapes and $\tau$ and quarkonium decays). In Ref. [2], we explore a more general procedure, in which the world-average data point on $\alpha_{s}\left(M_{Z}\right)$ is included in the fit in addition to the usual hadronic scattering data. A theoretical parameter for $\alpha_{s}\left(M_{Z}\right)$ is varied in this fit; its output value and uncertainty are determined by all input data. We find that the output value of $\alpha_{s}\left(M_{Z}\right)=0.118 \pm 0.0019$ obtained in this way essentially coincides with its input value $\alpha_{s}\left(M_{Z}\right)=0.118 \pm 0.002$. If the input value is not included, the output uncertainty on $\alpha_{s}$ is increased significantly, to $\alpha_{s}\left(M_{Z}\right)=0.118 \pm 0.005$. This indicates that the hadronic scattering data included in the fit imposes significantly weaker constraints on $\alpha_{s}$ than the other experiments contributing to the world-average value.

The Hessian PDF eigenvector sets returned by such floating- $\alpha_{s}$ fit can be used to estimate the correlation between the PDF parameters and $\alpha_{s}\left(M_{Z}\right)$. However, each of these eigenvector sets is inconveniently associated with its own value of $\alpha_{s}\left(M_{Z}\right)$. Instead, one can apply a simpler procedure, in which all eigenvector sets except two are determined for the best-fit value of $\alpha_{s}\left(M_{Z}\right)$. These eigenvector sets provide the usual PDF uncertainty for a fixed $\alpha_{s}\left(M_{Z}\right)$. Separately, the uncertainty in the PDFs induced by the uncertainty in $\alpha_{s}\left(M_{Z}\right)$ is assessed, by producing two alternative PDF fits for the $\alpha_{s}\left(M_{Z}\right)$ values at the lower and upper ends of the $\alpha_{s}$ uncertainty interval (i.e., $\alpha_{s}\left(M_{Z}\right)=0.116$ and 0.120$)$. These PDF and $\alpha_{s}$ uncertainties are then added in quadrature to obtain the total uncertainty.

This procedure is valid both formally and numerically. It is based on a theorem that is applicable within the quadratic approximation for the log-likelihood function $\chi^{2}$ in the vicinity of the best fit. The proof of the theorem, as well as a numerical demonstration of the equivalence of the addition in quadrature to the full estimation of the $\mathrm{PDF}+\alpha_{s}$ uncertainty based on the Hessian method, are given in Ref. [2]. The series of best-fit PDFs for $\alpha_{s}\left(M_{Z}\right)$ values in the interval 0.113-0.123, needed to evaluate the combined $\mathrm{PDF}+\alpha_{s}$ uncertainty in any application, are made available both for CTEQ6.6 and CT10 PDFs.

Figure 8: Left: Ratio of $g(x, Q)$ in SUSY fits with a fixed $\alpha_{s}\left(M_{Z}\right)=0.118$ and CT10 fit. Right: $\Delta \chi^{2}$ in 2004 and 2010 SUSY fits vs. gluino mass.


## Constraints on new physics from a global PDF analysis

Besides providing the PDFs and their uncertainties, the global QCD analysis can establish bounds on masses of hypothetical particles beyond the standard model (BSM), for example, relatively light color-octet Majorana fermions that contribute to strong interaction processes with the same coupling strength as the gluons. Gluinos of a supersymmetric (SUSY) origin serve as an example of such fermions; but other models can introduce them as well. Constraints on the "gluinos" are often imposed in the context of a specific BSM model for their production and decay, which helps to rule out "gluinos" with masses up to a few hundred GeV. But, if no model-specific assumptions are imposed, much lighter gluinos are allowed: as light as $\approx 12-15 \mathrm{GeV}$ according to the 2004 global fit based on the CTEQ6 set data [44], or $6-51 \mathrm{GeV}$ according to the NLO/resummation analyses of $e^{+} e^{-}$hadroproduction at LEP [45, 46, 47]. Note that the limit based on the global fit is not affected by (potentially important) theoretical uncertainties in the LEP analyses, associated with nonperturbative and matching effects in the resummation techniques that they employ.

In Ref. [48], we improve the earlier limits [44] on relatively light gluinos based on an extended CT10 fit with added gluino scattering contributions. In this study, an independent PDF describing gluinos, and one-loop splitting functions describing interactions of gluinos with quarks and gluons, are introduced in the DGLAP equation. Two-loop gluino contributions are included in the renormalization group equation for the running of $\alpha_{s}$. Cross sections for single-inclusive jet production are modified to include hard matrix elements for $2 \rightarrow 2$ processes involving gluinos, with full dependence on the gluino mass evaluated in the general-mass factorization scheme. These modifications capture the essential dependence on gluinos in inclusive processes studied in the CT10 fits. Generally, the gluino contributions to inclusive observables are small, so that they can be evaluated at the one-loop level to achieve the same accuracy as the SM contributions evaluated at two loops. Squarks and other BSM particles are assumed to be heavier than a few hundred GeV and not included.

Constraints on the gluino mass $m_{\tilde{g}}$ depend strongly on the value of $\alpha_{s}\left(M_{Z}\right)$ [44]. To reproduce the existing limits on $\alpha_{s}(Q)$, we introduce two data points at $Q=5 \mathrm{GeV}$ and $M_{Z}$, representing a combination of measurements at low $Q$ and $Q \approx M_{Z}$, respectively. The low- $Q$ bound on $\alpha_{s}$ has been obtained by combining measurements of $\alpha_{s}\left(M_{Z}\right)$ in $\tau$ and quarkonium decays. These low- $Q$
measurements are not affected by gluinos heavier than 10 GeV . Gluino contributions to the high- $Q$ data point are of the same order as the experimental uncertainties.

With the $\alpha_{s}$ data and latest hadronic data included, the 2010 SUSY PDF fits reduce the allowed range of gluino masses, as compared to the 2004 fits [44]. For example, Fig. 8 illustrates SUSY fits with a constant QCD coupling strength, $\alpha_{s}\left(M_{Z}\right)=0.118$, for gluino masses $m_{\tilde{g}}$ shown in the figure. The left subfigure compares the gluon PDF obtained in SUSY fits with $m_{\tilde{g}}=20$ and 50 GeV (solid lines) to the CT10 error band (corresponding to $m_{\tilde{g}}=\infty$ ). It is clear that too light gluinos distort the shape of the CT10 gluon PDF to an unacceptable level. The right subfigure shows the differences $\Delta \chi^{2}=\chi^{2}\left(\alpha_{s}, m_{\tilde{g}}\right)-\chi_{C T 10}^{2}$. One can see that $\Delta \chi^{2}>100$ for $m_{\tilde{g}}<25 \mathrm{GeV}$, suggesting that gluinos lighter than 25 GeV are excluded at about $90 \%$ C.L., for $\alpha_{s}\left(M_{Z}\right)=0.118$. This improves the 2004 constraint [44], $m_{\tilde{g}}>12 \mathrm{GeV}$ for $\alpha_{s}\left(M_{Z}\right)=0.118$, by a factor of two. Similarly, the 2004 limit on $m_{\tilde{g}}$ for a free $\alpha_{s}$, which allowed $m_{\tilde{g}}=1 \mathrm{GeV}$ for $\alpha_{s}\left(M_{Z}\right)=0.135$, is increased to $m_{\tilde{g}}>13 \mathrm{GeV}$ for any $\alpha_{s}$ in the 2010 fit.

Gluinos with mass about 50 GeV remain allowed both by the global fits and LEP data analysis. Such light gluinos may alter cross sections for jet production and other LHC processes [48]. We provide tables of PDFs with contributions of gluinos in this mass range to explore phenomenological implications.

Figure 9: Rapidity distributions of $W^{+}$and Higgs bosons computed with LO-MC and NLO PDF's.

## W+ rapidity distribution



## SM Higgs boson rapidity distribution




## PDFs for leading-order showering programs

Monte Carlo event generators, especially, the most mature leading-order generators, play a critical role in all stages of modern particle physics. Neither conventional LO PDFs, nor NLO PDFs produce satisfactory results when implemented in the showering programs. In Ref. [4], we modified the usual leading-order global analysis to find optimized PDFs for leading-order Monte-Carlo (LO-MC) simulations at the LHC. Besides the usual constraints from the existing hard-scattering experimental data, the joint input of this analysis incorporates pseudodata points for cross sections of $W, Z, t \bar{t}$, SM Higgs, and $g g \rightarrow b b^{\prime}$ production at the LHC, as predicted by NLO QCD theory. The PDFs resulting from this analysis are not strictly at the leading order: they include some information about key LHC processes evaluated at NLO. Event generators, including "LO event generators", have some elements of higher-order contributions and, in this sense, are not at the stated order in the QCD coupling. We can use their flexibility to find the LO-MC PDFs that better reproduce the benchmark NLO cross sections, when combined with LO matrix elements in a fixed-order calculation or a LO event generator.

To examine the available possibilities, we provide three representative LO-MC PDF sets, designated as CT09MCS, CT09MC1, and CT09MC2. These PDFs realize different strategies for bringing the LO predictions closer to NLO. Their differences stem from varying assumptions about the running of $\alpha_{s}$ (evaluated at one or two loops), factorization scales in the LHC pseudodata cross sections (fixed or fitted), and the momentum sum rule imposed on the PDFs (exact or relaxed by $10-15 \%$ [49]). An example of the LO-MC PDFs in action is shown in Fig.9, which compares cross sections for $W^{+}$boson and Standard Model Higgs boson rapidity distributions at the LHC, obtained with LO matrix elements and CT09MC2 and MRST2007lomod PDFs [49], and at NLO with CTEQ6.6. In the $W^{+}$production case (upper left subfigure), the CT09MC2 calculation closely reproduces both the normalization and shape of the NLO cross section at all three LHC energies, while the MRST2007lomod prediction differs from NLO in normalization at $\sqrt{s}=7 \mathrm{TeV}$, and both in normalization and shape at 10 and 14 TeV . For Higgs production (upper right subfigure), both CT09MC2 and MRST2007lomod predictions provide almost identical distributions, which are smaller than the NLO prediction by a nearly constant normalization factor. This difference with NLO reflects especially large virtual corrections present in Higgs production cross sections, which cannot be completely compensated by an increase in the LO gluon density. However, since the average normalization factors $K$ for each pseudodata process are also known from the fit (and published in our paper), end users can multiply the LO-MC cross sections for Higgs production and other pseudodata processes by these K-factors to better approximate the NLO cross sections (cf. the lower left subfigure). If an LHC process is not included as the pseudodata, comparison of LO predictions based on several LO-MC sets may still provide a reasonable estimate of the NLO cross section, as illustrated by the cross section for SM Higgs boson production via vector boson fusion in the lower right subfigure.

In summary, the CT10 and CT10W sets are based on the most up-to-date information about the PDFs available from global hadronic experiments. There are 26 free parameters in both new PDF sets; thus, there are 26 eigenvector directions and a total of 52 error PDFs for both CT10 and CT10W. The CT10 and CT10W PDF error sets, along with the accompanying $\alpha_{s}$ error sets, allow for a complete calculation of the combined $\mathrm{PDF}+\alpha_{s}$ uncertainties for any observable.

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# Correlated theoretical uncertainties for the one-jet inclusive cross section 

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#### Abstract

We discuss the correlated systematic theoretical uncertainties that may be ascribed to the next-toleading order QCD theory used to predict the one-jet inclusive cross section in hadron collisions. We estimate the magnitude of these errors as functions of the jet transverse momentum and rapidity. The total theoretical error is decomposed into a set of functions of transverse momentum and rapidity that give a model for statistically independent contributions to the error. This representation can be used to include the systematic theoretical errors in fits to the experimental data.


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## I. INTRODUCTION

Predictions of the standard model are typically made with the aid of next-to-leading order (NLO) perturbative calculations (or sometimes with NNLO calculations). Evidently, these predictions are not exactly equal to what one should measure if the standard model is correct. If we have an NLO calculation, we leave out NNLO and $\mathrm{N}^{3} \mathrm{LO}$ contributions, etc. We also leave out contributions that are suppressed by a power of the large momentum scale of the problem. Of course, we do not know exactly how big these contributions are: if we could calculate them, we would include them in the prediction. Nevertheless, we can estimate the size of the corrections. They then constitute "theory errors" in the prediction, which are quite similar to experimental systematic errors in the measurement.

In this paper we distinguish between errors associated with higher order contributions and power suppressed contributions to the cross section, which we call theory errors, and errors associated with our imperfect knowledge of the parton distribution functions needed for the prediction. Estimated theory errors are needed in two contexts. First, if an experiment does not agree with the theoretical prediction within the experimental statistical and systematic errors, then we need to see if there is agreement within the combined experimental and theory errors and the errors from the parton distributions used in the prediction. In the case that the disagreement is outside of the combined errors, then we have a signal for new physics.

The second context in which we need estimated theory errors is in the determination of parton distribution functions from experimental measurements. The theory errors give a contribution to the errors that we associate with the parton distribution functions that emerge from a fit to the data. Evidently, if we do not include theory errors, the resulting errors in the parton distribution functions will be too small. Additionally, if for one kind of process the

[^255]theory errors are large while for another kind of process the theory errors are small, then we will give the large-error process too much weight in the fit.

In this paper, we provide an estimate of the theory error for the one-jet inclusive cross section $d^{2} \sigma / d P_{T} d y$ in hadron-hadron collisions, where $P_{T}$ is the transverse momentum or "transverse energy" of the jet, and $y$ is the rapidity of the jet. There is good data for this process from the CDF and D0 experiments at Fermilab, including careful estimates of the experimental systematic errors. Estimates of the theory errors are needed to accompany the estimates of the experimental systematic errors.

We warn that there is no unique method to estimate theory errors. Thus our task is to provide a method that is defensible if not necessarily optimal. We seek to provide an estimate in a form that includes the correlations from one $\left\{P_{T}, y\right\}$ point to another.

## II. GENERAL SETUP

We treat theory errors in a fashion that is similar to that used for correlated systematic errors in the experimental results. We use next-to-leading order quantum chromodynamics (QCD) theory to make predictions for the one-jet inclusive cross section ${ }^{1}$

$$
\frac{d \sigma}{d P_{T} d y}=\int d x_{1} \int d x_{2} f_{a / A}\left(x_{1}, \mu\right) f_{b / B}\left(x_{2}, \mu\right) \frac{d \hat{\sigma}_{a b \rightarrow \mathrm{jet}}}{d P_{T} d y}
$$

In the calculation, one uses Monte Carlo integration so that there is a random statistical error for each point $\left\{P_{T}, y\right\}$. We do not include these statistical errors in the analysis here since they are typically quite small (say $2 \%$ ) and one can reduce them by running the program for a longer time. If we wished to include the errors from fluctuations in the Monte Carlo integrations, that task would be straightfor-

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FIG. 1 (color online). illustration of (a) uncorrelated and (b) correlated theoretical errors. In (a), the total error is about $10 \%$ for all $P_{T}$, but the error at any $P_{T}$ is not correlated with the error at nearby points. In (b), there are just three functions $f_{J}\left(P_{T}\right)$ giving, again, about a $10 \%$ total error at any one $P_{T}$. Because the $f_{J}\left(P_{T}\right)$ are smooth functions, the theoretical error at a given $P_{T}$ will be smoothly related to the error at other $P_{T}$ values.
ward because the statistical nature of these fluctuations is known.

We will start our investigation by studying jet production corresponding to the Tevatron Run 2, with $\sqrt{s}=$ 1960 GeV , as a function of $P_{T}$ and $y$. We will display the results for $y=\{0,1,2\}$ as functions of $P_{T}$; we also present formulas for the $P_{T}$ and $y$ dependence, from which estimated errors for the specific kinematic ranges used by CDF and D0 can be inferred.

We need estimated errors that can be used in a statistical analysis. However, we do not have at hand a statistical ensemble of worlds in which terms beyond those included in the NLO theory vary. Thus we make estimates that we hope are reasonable but that can and should be subject to debate.

We formulate the treatment of theory errors as follows. We let

$$
\begin{equation*}
\frac{d \sigma}{d P_{T} d y}=\left[\frac{d \sigma}{d P_{T} d y}\right]_{\mathrm{NLO}}\left\{1+\sum_{J} \lambda_{J} f_{J}\left(P_{T}, y\right)\right\} . \tag{1}
\end{equation*}
$$

Here the functions $f_{J}\left(P_{T}, y\right)$ are definite functions, while the $\lambda_{J}$ are unknown parameters. Thus $\lambda_{J} f_{J}\left(P_{T}, y\right)$ represents an unknown theoretical contribution that might modify the NLO theory. We treat the $\lambda_{J}$ as Gaussian random variables with variance 1 . That is, the size of the uncertainty with label $J$ is represented by how $\operatorname{big} f_{J}\left(P_{T}, y\right)$ is. If one thinks of this as representing an imaginary ensemble of worlds in which theory calculations come out differently, then these worlds all have the same $f_{J}$ but the $\lambda_{J}$ vary.

We will propose to use just a few functions $f_{J}$. We offer the following defense of this strategy. Consider a simplified case of a cross section that is a function of just one variable, $P_{T}$. If we were to believe that the uncertainty in the prediction of this cross section is of order, say, $10 \%$, but we have no idea of what the shape of the true cross section is within a $10 \%$ band about the prediction, then we would choose many functions $f_{J}\left(P_{T}\right)$, each of size 0.10 , but with
each being nonzero only in a very tiny range of $P_{T}$. This approach is illustrated in Fig. 1(a); such a view seems to us unreasonable.

Experience with various perturbative and nonperturbative contributions teaches that they are smooth functions of the relevant variables, $P_{T}$ in this case. This arguably more reasonable scenario is illustrated in Fig. 1(b). As illustrated by the three curves, ${ }^{2}$ one contribution beyond NLO could be flat, amounting to a constant " K factor," another might be a smoothly increasing function of $P_{T}$, while yet another might be positive at high and low $P_{T}$ and negative in between. However, we judge it unlikely that a currently uncalculated contribution would have multiple maxima between low and high $P_{T}$.

Thus we seek a few functions $f_{J}\left(P_{T}, y\right)$ that have some dependence on $\left\{P_{T}, y\right\}$ and represent, as best we can determine, our understanding of the character of uncalculated contributions. In the following sections, we analyze several sources of theory errors and associate them with functions $f_{J}\left(P_{T}, y\right)$.

## III. PERTURBATIVE UNCERTAINTY

The main source of uncertainty at large jet transverse momentum, at least in our estimation, is the fact that we have calculated only at NLO, leaving contributions from higher orders of perturbation uncalculated. We estimate this uncertainty using the dependence of the computed cross section on the renormalization and factorization scales. We present this estimate in this section. In the

[^257]following section, we check this estimate using an independent method involving threshold effects.

## A. Error estimate from scale dependence

The first ingredient in our estimation of theory errors is based on the traditional method in which one evaluates the dependence of the computed NLO cross section on two scales: the renormalization scale $\mu_{\mathrm{R}}$ and the factorization scale $\mu_{\mathrm{F}}$. One often makes a standard choice for these scales: $\mu_{\mathrm{R}}=\mu_{\mathrm{F}}=P_{T} / 2$. We will take this choice as our central value and define

$$
\begin{equation*}
x_{1}=\log _{2}\left(\frac{\mu_{\mathrm{R}}}{P_{T} / 2}\right), \quad x_{2}=\log _{2}\left(\frac{\mu_{\mathrm{F}}}{P_{T} / 2}\right) \tag{2}
\end{equation*}
$$

We compute the cross section near $x_{1}=x_{2}=0$, that is near the scale choice $\mu_{\mathrm{R}}=\mu_{\mathrm{F}}=P_{T} / 2$. Then $\left\{x_{1}, x_{2}\right\}$ measures (logarithmically) the distance from this central value. We then fit the cross section to a quadratic polynomial $P(\vec{x})$ in $\vec{x}$-space,

$$
\begin{equation*}
\left[\frac{d \sigma\left(x_{1}, x_{2}\right)}{d P_{T}}\right]_{\mathrm{NLO}} \approx\left[\frac{d \sigma(0,0)}{d P_{T}}\right]_{\mathrm{NLO}}[1+P(\vec{x})] \tag{3}
\end{equation*}
$$

where

$$
\begin{equation*}
P(\vec{x})=\sum_{J} x_{J} A_{J}+\sum_{J, K} x_{J} M_{J K} x_{K}, \tag{4}
\end{equation*}
$$

with $\vec{x}=\left(x_{1}, x_{2}\right)$ and $J, K=\{1,2\}$.
We know that if we had an NNLO calculation, the dependence of the cross section on $\vec{x}$ would be canceled to order $\alpha_{s}^{2}$. Thus the coefficients $A_{J}$ and $M_{J K}$ carry information about the perturbative coefficients beyond NLO. For this reason, we use the coefficients $A_{J}$ and $M_{J K}$ to provide an estimate of the error induced by truncating the perturbative expansion at one-loop order. We define a simple recipe for this purpose. We define an estimated error ${ }^{3} \mathcal{E}_{\text {scale }}$ as the root-mean-square average of $P(\vec{x})$ over a circle with a certain radius $|\vec{x}|$,

$$
\begin{equation*}
\mathcal{E}_{\text {scale }}^{2}=\frac{1}{2 \pi} \int_{0}^{2 \pi} d \theta P(|\vec{x}| \cos \theta,|\vec{x}| \sin \theta)^{2} \tag{5}
\end{equation*}
$$

We need to select a value of $|\vec{x}|$, and we make the choice

$$
\begin{equation*}
|\vec{x}|=2 \tag{6}
\end{equation*}
$$

In the most common method of estimating errors from scale variation, we would vary $\left(2 \mu_{\mathrm{R}} / P_{T}, 2 \mu_{\mathrm{F}} / P_{T}\right)$ between $(1,1)$ and $(2,2)$ and between $(1,1)$ and $(1 / 2,1 / 2)$. This amounts to changing $\vec{x}$ from 0 to a vector of length $|\vec{x}|=\sqrt{2}$ in a particular direction that corresponds to something close to the direction of strongest variation. The choice $|\vec{x}|=2$ is somewhat larger than this standard choice. For instance, $|\vec{x}|=2$ in the direction $\vec{x} \propto(1,1)$

[^258]corresponds to
\[

$$
\begin{equation*}
\left(\frac{\mu_{\mathrm{R}}}{P_{T} / 2}, \frac{\mu_{\mathrm{F}}}{P_{T} / 2}\right)=\left(2^{\sqrt{2}}, 2^{\sqrt{2}}\right) \approx(2.7,2.7) \tag{7}
\end{equation*}
$$

\]

We average over the directions of $\vec{x}$ instead of taking a particular direction. For this reason, the value of Eq. (6) gives results that are similar to the method that is often used. While varying the $\mu$-scales along the $(1,1)$ direction will often work, our averaging technique provides a general method that seems sensible even when the one of the directions of slowest variation happens to align with the $(1,1)$ direction.

A straightforward calculation shows that, with the definition (5),

$$
\begin{equation*}
\mathcal{E}_{\text {scale }}^{2}=\frac{|\vec{x}|^{2}}{2} \vec{A}^{2}+\frac{|\vec{x}|^{4}}{8}\left[(\operatorname{Tr} M)^{2}+2 \operatorname{Tr} M^{2}\right] \tag{8}
\end{equation*}
$$

We determine the coefficients $A_{J}$ and $M_{J K}$ by calculating the one-jet inclusive cross section for a given value of $P_{T}$ and rapidity. We use nine points in $\vec{x}$-space, obtained by setting each $\left\{\mu_{\mathrm{R}}, \mu_{\mathrm{F}}\right\}$ scale to $\left\{\frac{1}{4} P_{T}, \frac{1}{2} P_{T}, P_{T}\right\}$ and fit the results to the form given in Eqs. (3) and (4).

## B. Contour plots

We illustrate this procedure for estimating the theoretical error from this source in Fig. 2, where we display contour plots of $1+P(\vec{x})$ corresponding to the jet cross section at the Tevatron with $P_{T}=100 \mathrm{GeV}$ for $y=0$ and for $y=2$. For both values of $y$, we find a saddle point in the vicinity of $\left\{x_{1}, x_{2}\right\}=\{0,0\}$ which corresponds to $\left\{\mu_{\mathrm{R}}, \mu_{\mathrm{F}}\right\}=\left\{P_{T} / 2, P_{T} / 2\right\}$. This location of the saddle point is a general feature that holds throughout much of the kinematic range; it motivates the choice $\left\{\mu_{R}, \mu_{\mathrm{F}}\right\}=$ $\left\{P_{T} / 2, P_{T} / 2\right\}$ as our central values.

The estimated scale dependence error, $\mathcal{E}_{\text {scale }}$, is then obtained by averaging the deviation of the cross section at a given radius in $\vec{x}$-space. As discussed above, we choose a radius of $|\vec{x}|=2$, as indicated by the circle in Fig. 2. The slope of the $\left\{x_{1}, x_{2}\right\}$ surface is steeper for the $y=2$ case as compared with the $y=0$ case. Consequently, we find a larger $\mathcal{E}_{\text {scale }}$ for $y=2(\sim 18 \%)$ as compared to $y=0(\sim$ $9 \%$ ).

## C. Comment on the range of scale choices

In the above analysis, we estimate the theoretical uncertainty by varying the $\mu$ scales by a factor about a central value. This is a conventional choice, but is it reasonable? To examine this question, one can look at cases in which NNLO calculations exist. Here, we choose one typical case as an example. In Fig. 3, we show the NNLO cross section for Higgs production at the Large Hadron Collider (LHC) as a function of the $P_{T}^{\text {veto }}$ parameter as calculated by Ref. [2]. Here, the renormalization and factorization scales are varied by a factor of $2,\left\{\mu_{\mathrm{R}}, \mu_{\mathrm{F}}\right\} \in\left[M_{\mathrm{h}} / 2,2 M_{\mathrm{h}}\right]$.


FIG. 2 (color online). Contour plot of the jet cross section in the $\left\{x_{1}, x_{2}\right\}$ plane for the Tevatron $(\sqrt{s}=1960 \mathrm{GeV})$ with $P_{T}=$ 100 GeV and (a) central rapidity $y=0$ and (b) forward rapidity $y=2$. We plot the ratio of the cross section compared to the central value at $\left\{x_{1}, x_{2}\right\}=\{0,0\}$. Contour lines are drawn at intervals of 0.10. The (red) circle is at radius $|x|=2$.

Consider, for example, $P_{T}^{\text {veto }}$ near 80 GeV . To simplify our argument, let us suppose that the exact QCD result is known and that it lies in the middle of the NNLO error band. We then ask whether the estimated NLO error band was reasonable, now that we know the exact answer. To do a real statistical analysis, we should have at hand many NLO calculations of separate and independent quantities, each with its error estimate. For each such quantity, a NNLO calculation that we can regard as nearly "exact" should be available. We would then plot the distribution of the differences between the NLO central value and the true answer in units of the NLO $1 \sigma$ error estimate. If the error estimates are reliable, this distribution should be a Gaussian distribution with width 1 . We cannot do that with just one datum. However, we can say that if the

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FIG. 3 (color online). The cross section for Higgs production at the LHC for LO, NLO, and NNLO calculations as taken from Ref. [2]. The computed cross section vetos jets $\left(P_{T}^{\text {jet }}>P_{T}^{\text {veto }}\right)$ in the central region $|\eta|<2.5$.

NLO estimate is reasonable then the central NNLO value in the one case that we have should be roughly $1 \sigma$ away from the NLO central value. If it is $3 \sigma$ away, then it seems likely that the NLO error was underestimated. If it is $0.1 \sigma$ away, then seems likely that the NLO error was overestimated. In the case at hand, the difference is about $1 \sigma$, so we have some evidence that the error was correctly estimated.

## D. Scale dependence total uncertainty

Implementing the procedure outlined above, we find the theoretical systematic error estimated from scale dependence, $\mathcal{E}_{\text {scale }}$; this is displayed in Fig. 4. The (blue) points are $\mathcal{E}_{\text {scale }}$ computed as described above from the NLO cross section [1] and the (red) curve is a smooth fit to these points.

We see that $\mathcal{E}_{\text {scale }}\left(P_{T}, y\right)$, is a slowly rising function of $P_{T}$. For the rapidity $y=0$ at the Tevatron $(\sqrt{s}=$ 1960 GeV ), we find that $\mathcal{E}_{\text {scale }}\left(P_{T}, y\right)$ varies from $9 \%$ to $11 \%$. For $y=1$, the uncertainty ranges from $9 \%$ to $20 \%$, and for $y=2$ the uncertainty increases even more, ranging from $12 \%$ to $25 \%$ over a more limited $P_{T}$ range.

## E. Scale dependence correlated uncertainty

As described in Sec. II, we decompose the total scale dependence uncertainty, $\mathcal{E}_{\text {scale }}$, into a (small) number of functions $f_{J}\left(P_{T}, y\right)$ which then combine to form the total uncertainty $\mathcal{E}_{\text {scale }}$.

Since the $f_{J}\left(P_{T}, y\right)$ functions represent independent sources of uncertainty, $\mathcal{E}_{\text {scale }}$ is the quadrature sum

$$
\begin{equation*}
\mathcal{E}_{\text {scale }}\left(P_{T}, y\right) \equiv \sqrt{\sum f_{J}\left(P_{T}, y\right)^{2}} \tag{9}
\end{equation*}
$$

We chose a set of functions $f_{J}\left(P_{T}, y\right)$ that satisfies Eq. (9).




FIG. 4 (color online). The estimate of the uncertainty $\mathcal{E}\left(P_{T}, y\right)=\mathcal{E}_{\text {scale }}$ due to the scale variation as given in Eq. (8) for the Tevatron $(\sqrt{s}=1960 \mathrm{GeV})$ with $y=\{0,1,2\}$. The calculation from the jet code is represented by the (blue) points, and the fit based on Eq. (9) is shown with the solid (red) curve.


FIG. 5 (color online). The estimate of the uncertainty $\mathcal{E}_{\text {scale }}$ due to the scale variation as given in Eq. (8) for the Tevatron ( $\sqrt{s}=$ 1960 GeV ) with $y=\{0,1,2\}$. The combined uncertainty $\mathcal{E}_{\text {scale }}$ is shown as the upper thick (red) curve, and the individual functions $f_{J}\left(P_{T}, y\right)$ are indicated below.

We take the $f_{J}\left(P_{T}, y\right)$ to depend on $y$ and on the ratio of $P_{T}$ to the quantity ${ }^{4}$

$$
\begin{equation*}
M(y)=\sqrt{s} e^{-y} \tag{10}
\end{equation*}
$$

For the set of $f_{J}\left(P_{T}, y\right)$ functions we choose

$$
\begin{align*}
& f_{1}\left(P_{T}, y\right)=\frac{9.62 \times 10^{-2}}{\log \left(M(y) / P_{T}\right)}, \\
& f_{2}\left(P_{T}, y\right)=\frac{2.89 \times 10^{-2} y^{2}}{\log \left(M(y) / P_{T}\right)}, \\
& f_{3}\left(P_{T}, y\right)=8.42 \times 10^{-2},  \tag{11}\\
& f_{4}\left(P_{T}, y\right)=0.842 \times 10^{-2} y^{2}, \\
& f_{5}\left(P_{T}, y\right)=1.68 \times 10^{-2} \log \left(\frac{15 P_{T}}{M(y)}\right) \\
& f_{6}\left(P_{T}, y\right)=0.336 \times 10^{-2} y^{2} \log \left(\frac{15 P_{T}}{M(y)}\right) .
\end{align*}
$$

[^259]These functions are illustrated in Fig. 5. The first two terms are singular as $P_{T} \rightarrow M(y)$. The first controls the singular behavior near $y=0$ while the second modifies the singular behavior for large $y$. The remaining terms constitute a polynomial in $\log \left(P_{T}\right)$ and $y^{2}$. Thus, we parametrize the $y$-dependence with the set of functions $\left\{1, y^{2}\right\}$, and the $P_{T}$-dependence with the set of functions $\{1 / L, 1, L\}$ where $L$ represents a logarithmic function of $P_{T}$. We believe that the parametrization in terms of these $2 \times 3=6$ functions is sufficient to reasonably describe the theoretical uncertainties.

Note that the coefficients of $f_{3}$ and $f_{4}$ are in the ratio $10: 1$ and the coefficients of $f_{5}$ and $f_{6}$ are in the ratio 5:1. While we could find an excellent fit without $f_{4}$ and $f_{6}$, we retain these terms to provide flexibility when one tries to fit the $\lambda_{J}$ coefficients to actual data.

We can perform a similar exercise for the LHC as well; these results will be compiled and presented in Sec. VII.

## IV. SUMMATION OF THRESHOLD LOGS

For parton-parton scattering near the threshold for the production of a jet with a given $P_{T}$, there is restricted phase space for real gluon emission. Thus, there is an incomplete


FIG. 6 (color online). The ratio of the two-loop threshold resummation contributions for jet production compared to the total NLO cross section $\sigma_{\text {resum }} / \sigma_{\text {NLO }}$ at the Tevatron $(\sqrt{s}=$ 1960 GeV ) vs $P_{T}$ in GeV . We have set the scales to $\mu_{\mathrm{F}}=\mu_{\mathrm{R}}=$ $P_{T} / 2$, and used $y=0$. The points are computed using the implementation of the 2-loop threshold resummation by Kidonakis and Owens [9].
cancellation of infrared divergences between real and virtual graphs, resulting in large logarithms $L$ inside the integration over parton momentum fractions. At $n$th order in $\alpha_{\mathrm{s}}$ these logarithms enter the cross section in the general form $\alpha_{\mathrm{s}}^{n} L^{2 n}$. The leading logarithms can be summed to all orders in $\alpha_{\mathrm{s}}$. We make use of the numerical results from Ref. [3], which has been implemented in the FASTNLO program [4].

Figure 6 displays the size of the threshold correction for Tevatron jet measurements at $y=0$. The curve is presented for the scale choice $\mu=P_{T} / 2$; we note that for this scale choice, the threshold correction is generally smaller than with other scale choices. ${ }^{5}$

We find the threshold corrections in this kinematic regime to be less than those discussed in the previous section (Sec. III) and shown in Fig. 5. As the threshold corrections also arise from uncomputed higher-order terms, these corrections are, in a sense, already accommodated by the larger uncertainty that we estimated from scale variation in Eq. (11). Indeed, the functions $f_{J}$ for $J=1$ and $J=2$ contain singularities for $P_{T} \rightarrow M(y)$ that are meant to incorporate the threshold singularities. For this reason, we will not add a separate $f_{J}\left(P_{T}, y\right)$ function in the expression for the total uncertainty $\mathcal{E}$ to represent the effects of threshold logarithms.

[^260]
## V. UNDERLYING EVENT AND HADRONIZATION

A separate source of uncertainties in jet measurements comes from what is colloquially known as "splash-in" and "splash-out" corrections. "Splash-in" corrections arise from the underlying event, which can deposit additional energy into the jet cone; we will refer to these more formally as underlying event (UE) corrections. "Splashout" corrections come from the hadronization process of the jet which may move some of the jet energy outside the defined jet cone. We will refer to these as hadronization corrections (HC).

In either case, the correction is modeled as adding an amount $\delta P_{T}$ to the observed transverse momentum (or transverse energy) of the jet. We denote the average over many events of $\delta P_{T}$ by $\left\langle\delta P_{T}\right\rangle$. A complete analysis of the UE and HC contributions was performed by Cacciari, Dasgupta, Magnea, Salam in Refs. [5-7]. We find this to be an entirely suitable method for our estimate of $\left\langle\delta P_{T}\right\rangle$, and we adapt their results in the following.

## A. Underlying event (UE)

We can parametrize the effect of the underlying event corrections on the apparent $P_{T}$ of the jet as

$$
\begin{equation*}
\left\langle\delta P_{T}\right\rangle_{\mathrm{UE}}=\Lambda_{\mathrm{UE}} \frac{1}{2} R^{2} \tag{12}
\end{equation*}
$$

where $R$ is the cone radius of the jet and $\Lambda_{\mathrm{UE}}$ is the average transverse energy per unit rapidity in the underlying event. Because we model the "splash-in" energy as random and uncorrelated with how the jet develops, the contribution from the underlying event will scale as the area of the jet cone-hence the factor of $R^{2}$ in Eq. (12). At Tevatron energies, Ref. [5] finds

$$
\begin{equation*}
\Lambda_{\mathrm{UE}}(1960 \mathrm{GeV}) \approx 3 \pm 1 \mathrm{GeV} \tag{13}
\end{equation*}
$$

Thus, the $\left\langle P_{T}\right\rangle$ shift from the underlying event corrections is given by

$$
\begin{equation*}
\left\langle\delta P_{T}\right\rangle_{\mathrm{UE}} \approx+0.7 \mathrm{GeV} \pm 0.3 \mathrm{GeV} \tag{14}
\end{equation*}
$$

for a jet cone with $R=0.7$.

## B. Hadronization correction (HC)

The $R$ dependence of hadronization correction is very different from that of the underlying event correction [57]. The smaller the jet cone is, the more likely it is that hadronization will spray hadrons out of the cone. Hence, we will parametrize these corrections as proportional to $1 / R$. Following Ref. [5], we write the hadronization correction as

$$
\begin{equation*}
\left\langle\delta P_{T}^{i}\right\rangle_{\mathrm{HC}}=-C_{i} \frac{2}{R} \mathcal{A}\left(\mu_{I}\right) \tag{15}
\end{equation*}
$$

where $\mathcal{A}\left(\mu_{I}\right)$ parametrizes the soft gluon radiation. Reference [5] takes $\mu_{I}=2 \mathrm{GeV}$, and finds $\mathcal{A}(2 \mathrm{GeV}) \approx$ 0.2 GeV . In Eq. (15), $C_{i}$ is a color factor that depends on
whether the jet is initiated by a quark, for which $C_{i}=$ $C_{\mathrm{F}}=4 / 3$, or by a gluon, for which $C_{i}=C_{\mathrm{A}}=3$. We thus need an estimate of the fraction of jets that are gluon jets. Using calculations from the literature [8], we estimate that, for the Tevatron in the low $P_{T}$ region, the fractions of quark and gluon jets are approximately

$$
f_{q} \approx \frac{2}{3}, \quad f_{g} \approx \frac{1}{3}
$$

Using these fractions, we can form a weighted average of the quark and gluon terms to obtain

$$
\begin{align*}
\left\langle\delta P_{T}\right\rangle_{\mathrm{HC}} & =f_{q}\left\langle\delta P_{T}^{q}\right\rangle_{\mathrm{HC}}+f_{g}\left\langle\delta P_{T}^{g}\right\rangle_{\mathrm{HC}} \\
& =-f_{q} \frac{2 C_{\mathrm{F}}}{R} \mathcal{A}\left(\mu_{I}\right)-f_{g} \frac{2 C_{\mathrm{A}}}{R} \mathcal{A}\left(\mu_{I}\right) \\
& \approx-1 \mathrm{GeV} \pm 0.5 \mathrm{GeV} . \tag{16}
\end{align*}
$$

Here, we have used a typical cone radius of $R=0.7$ and taken a conservative choice for the uncertainty of $50 \%$ of the correction.

## C. $\left\langle\delta P_{T}\right\rangle$ from the UE and HC

Combining the underlying event of Eq. (14) and the hadronization corrections of Eq. (16), the net $P_{T}$ shift is

$$
\begin{equation*}
\left\langle\delta P_{T}\right\rangle \approx-0.3 \mathrm{GeV} \pm 0.6 \mathrm{GeV} \tag{17}
\end{equation*}
$$

where we have added the separate uncertainties in quadrature.

The individual underlying event and hadronization results for $\left\langle\delta P_{T}\right\rangle$ are displayed in Fig. 7 for the Tevatron using the parametrizations of Eq. (14) and (16). The combined result for $\left\langle\delta P_{T}\right\rangle$, including the uncertainty band, is also displayed. The underlying event and hadronization


FIG. 7 (color online). We display the expected $P_{T}$ shift, $\left\langle\delta P_{T}\right\rangle$, in GeV vs jet cone radius $R$ for the UE, HC, and combined results (TOT) at the Tevatron. The calculation of the HC uses a combination of quark-initiated $\left(f_{q}=2 / 3\right)$ and gluon-initiated $\left(f_{g}=1 / 3\right)$ jets. The upper solid (blue) line represents the UE correction, and the lower solid (green) line represents the HC terms. The combination of these corrections (TOT) is represented by the central (red) band including the uncertainties. The vertical line corresponds to $R=0.7$.
corrections have opposite sign, and we note that for a jet cone radius of $R=0.7$, the two corrections nearly cancel each other.

## D. From $\left\langle\delta P_{\boldsymbol{T}}\right\rangle$ to $\boldsymbol{\delta} \boldsymbol{\sigma}$

The differential jet cross section can be approximated by a power law of the form

$$
\begin{equation*}
\frac{d \sigma\left(P_{T}\right)}{d P_{T}} \approx \frac{\mathrm{const}}{P_{T}^{n}} \tag{18}
\end{equation*}
$$

in the specific $P_{T}$ range of interest. For jets at the Tevatron in the intermediate $P_{T}$ range of $\sim[50,300] \mathrm{GeV}$, we find $n \approx 7$ as illustrated by Fig. 8.

The effect of the underlying event and hadronization corrections is to shift the jet $P_{T}$ from its value $P_{T}^{\text {pert }}$ at the NLO parton level to a new value

$$
P_{T}=P_{T}^{\text {pert }}+\left\langle\delta P_{T}\right\rangle,
$$

where $\left\langle\delta P_{T}\right\rangle$ is the average change in the transverse jet transverse momentum due to underlying event additions and hadronization subtractions from Eq. (17).

If we write the true differential cross section as a function $f$,

$$
\frac{d \sigma\left(P_{T}\right)}{d P_{T}} \equiv f\left(P_{T}\right)
$$

then $f$ is related to the perturbatively calculated function $f_{\text {pert }}$ by

$$
f\left(P_{T}\right) \approx f_{\text {pert }}\left(P_{T}^{\text {pert }}\right)=f_{\text {pert }}\left(P_{T}-\left\langle\delta P_{T}\right\rangle\right)
$$

We can perform a Taylor expansion about $P_{T}$ for small $\delta P_{T}$,


FIG. 8 (color online). Jet cross section $d^{2} \sigma / d P_{T} / d y$ vs $P_{T}$ in GeV with $y=0$ at the Tevatron in units of $\mathrm{nb} / \mathrm{GeV}$. The line is a power law fit with $n=7$; this describes the slope of the jet data in the range $P_{T} \approx[50,300] \mathrm{GeV}$.

$$
\begin{aligned}
f\left(P_{T}\right) & \approx f_{\text {pert }}\left(P_{T}-\left\langle\delta P_{T}\right\rangle\right) \\
& \approx f_{\text {pert }}\left(P_{T}\right)-\left\langle\delta P_{T}\right\rangle \frac{d f_{\text {pert }}^{\prime}\left(P_{T}\right)}{d P_{T}} \\
& =f_{\text {pert }}\left(P_{T}\right)\left\{1+n \frac{\left\langle\delta P_{T}\right\rangle}{P_{T}}\right\} .
\end{aligned}
$$

Here we have used the power law of Eq. (18) to replace $f^{\prime}\left(P_{T}\right)$ by $-n f\left(P_{T}\right) / P_{T}$. Thus, to first order we find ${ }^{6}$

$$
\begin{equation*}
\frac{d \sigma}{d P_{T}} \approx \frac{d \sigma_{\mathrm{pert}}}{d P_{T}}\left[1+n \frac{\left\langle\delta P_{T}\right\rangle}{P_{T}}+\cdots\right] \tag{19}
\end{equation*}
$$

so that the fractional correction is $n\left\langle\delta P_{T}\right\rangle / P_{T}$. Using $n \approx$ 7 and the estimate from Eq. (17) of $\left\langle\delta P_{T}\right\rangle$, we find that the fractional correction to the cross section is approximately

$$
7 \times \frac{-0.3 \mathrm{GeV} \pm 0.6 \mathrm{GeV}}{P_{T}} \approx-\frac{2 \mathrm{GeV}}{P_{T}} \pm \frac{4 \mathrm{GeV}}{P_{T}}
$$

Thus we estimate the fractional uncertainty from the underlying event and hadronization to be $4 \mathrm{GeV} / P_{T}$.

We account for this source of uncertainty by adding a new function $f_{J}\left(P_{T}, y\right)$ with $J=7$,

$$
\begin{equation*}
f_{7}\left(P_{T}, y\right)=\frac{4 \mathrm{GeV}}{P_{T}} \tag{20}
\end{equation*}
$$

for Tevatron jets in the $P_{T}$ range of $\sim[50,300] \mathrm{GeV}$.

## VI. SUMMARY FOR THE TEVATRON

We have described the correlated theoretical systematic uncertainty using a total of seven functions, as summarized in Table I. The net error at any one value of $\left\{P_{T}, y\right\}$ is obtained by adding these seven functions in quadrature

$$
\begin{equation*}
\mathcal{E}\left(P_{T}, y\right) \equiv \sqrt{\sum f_{J}\left(P_{T}, y\right)^{2}} \tag{21}
\end{equation*}
$$

We now summarize the complete set of contributions to the uncertainty of the differential jet cross section as a function of $\left\{P_{T}, y\right\}$ for the Tevatron:
$f_{1}\left(P_{T}, y\right)=\frac{9.62 \times 10^{-2}}{\log \left(M(y) / P_{T}\right)}, \quad f_{2}\left(P_{T}, y\right)=\frac{2.89 \times 10^{-2} y^{2}}{\log \left(M(y) / P_{T}\right)}$
$f_{3}\left(P_{T}, y\right)=8.42 \times 10^{-2}, \quad f_{4}\left(P_{T}, y\right)=0.842 \times 10^{-2} y^{2}$,
$f_{5}\left(P_{T}, y\right)=1.68 \times 10^{-2} \log \left(\frac{15 P_{T}}{M(y)}\right)$,
$f_{6}\left(P_{T}, y\right)=0.336 \times 10^{-2} y^{2} \log \left(\frac{15 P_{T}}{M(y)}\right)$,
$f_{7}\left(P_{T}, y\right)=\frac{4 \mathrm{GeV}}{P_{T}}$.
We display these results in Fig. 9. For $P_{T} \gtrsim 100 \mathrm{GeV}$, the perturbative uncertainties are dominant, and slowly rise

[^261]TABLE I. A compilation of the source of uncertainties $\left(f_{J}\right)$ that comprise the total jet cross section uncertainty $\mathcal{E}$. The perturbative uncertainties arise from the higher, uncalculated, orders of perturbation theory and are estimated using the $\left\{\mu_{\mathrm{F}}, \mu_{\mathrm{R}}\right\}$ scale variation of the calculated cross section. The nonperturbative uncertainties are an estimate of the underlying event and hadronization corrections.

| Uncertainty $f_{J}$ | Source |
| :--- | :---: |
| $\left\{f_{1}, f_{2}, f_{3}, f_{4}, f_{5}, f_{6}\right\}$ | perturbative |
| $f_{7}$ | nonperturbative |

with increasing $P_{T}$; this results holds across the full $y$-range, but the rise with $P_{T}$ is more pronounced at large $y$. For $P_{T} \lesssim 100 \mathrm{GeV}$, the uncertainty from the UE and HC terms become increasingly important as $P_{T}$ decreases.

## VII. THEORY ERRORS AT THE LHC

Having demonstrated the method for determining the theoretical systematic uncertainty at the Tevatron, we perform a parallel analysis for the Large Hadron Collider (LHC).

## A. Perturbative uncertainty

We again estimate the error from not having calculated beyond NLO by using the dependence of the NLO cross section on the scales $\left\{\mu_{\mathrm{R}}, \mu_{\mathrm{F}}\right\}$, just as in the Tevatron case, and this yields the functions $\left\{f_{1}, f_{2}, f_{3}, f_{4}, f_{5}, f_{6}\right\}$ summarized in Eq. (27) at the end of this section.

## B. Underlying event and hadronization

We proceed as in Sec. V for the Tevatron, accounting for the changed circumstances at the LHC. We first need to estimate the error in the determination of the contribution to the average jet transverse momentum, $\left\langle\delta P_{T}\right\rangle$, arising from the underlying event and from hadronization.

The underlying event contribution to $\left\langle\delta P_{T}\right\rangle$ is determined by the parameter $\Lambda_{\mathrm{UE}}$ in Eq. (12). Consistently with Refs. [5-7], for the LHC we take $\Lambda_{\mathrm{UE}}(14 \mathrm{TeV}) \approx$ $10 \pm 4 \mathrm{GeV}$, and obtain

$$
\begin{equation*}
\left\langle\delta P_{T}\right\rangle_{\mathrm{UE}} \approx+2.5 \mathrm{GeV} \pm 1 \mathrm{GeV} \tag{23}
\end{equation*}
$$

For the contribution to $\left\langle\delta P_{T}\right\rangle$ from hadronization, we use Eq. (16) with $\mathcal{A}\left(\mu_{I}\right) \approx 0.2 \mathrm{GeV}$ as before. For the fractions $f_{q}$ and $f_{g}$ of quark and gluon jets in the relatively low $P_{T}$ region where the hadronization corrections are significant, we use

$$
f_{q} \approx \frac{1}{3}, \quad f_{g} \approx \frac{2}{3} .
$$

Using these fractions, we can form a weighted average of the quark and gluon terms and estimate the hadronization contribution to $\left\langle\delta P_{T}\right\rangle$ to be

$$
\begin{equation*}
\left\langle\delta P_{T}\right\rangle_{\mathrm{HC}}=-1.4 \mathrm{GeV} \pm 0.7 \mathrm{GeV} \tag{24}
\end{equation*}
$$



FIG. 9 (color online). A compilation of the uncertainties for jet production at the Tevatron $(\sqrt{s}=1960 \mathrm{GeV})$ for $y=\{0,1,2\}$. The numeric label corresponds to the error components summarized in Eq. (27). The upper thick (red) line is the quadrature sum of the individual errors.

Combining the underlying event and hadronization contributions, we estimate

$$
\begin{equation*}
\left\langle\delta P_{T}\right\rangle \approx+1 \mathrm{GeV} \pm 1.2 \mathrm{GeV} \tag{25}
\end{equation*}
$$

where we have added the separate uncertainties in quadrature.

The results for the underlying event and hadronization contribution to $\left\langle\delta P_{T}\right\rangle$ are displayed in Fig. 10 for the LHC using the parametrizations of Eq. (24) and (23) but with a variable cone size $R$.

The correction to $\left\langle\delta P_{T}\right\rangle$ determines the correction to the cross section via Eq. (19). For this, we need the power $n$ that describes the approximate power law fall off of the cross section. As illustrated in Fig. 11, a power law with $n \approx 6$ describes the data over the range $P_{T} \approx$ $[100,1000] \mathrm{GeV}$. Using $n \approx 6$ and the estimate from Eq. (25) of $\left\langle\delta P_{T}\right\rangle$, we find that the fractional correction to the cross section is approximately


FIG. 10 (color online). We display the expected $P_{T}$ shift, $\left\langle\delta P_{T}\right\rangle$, in GeV vs jet cone radius $R$ for the $\mathrm{UE}, \mathrm{HC}$, and combined results (TOT) at the LHC. The calculation of the HC uses a combination of quark-initiated $\left(f_{q}=1 / 3\right)$ and gluon-initiated ( $f_{g}=2 / 3$ ) jets. The upper solid (blue) line represents the UE correction, and the lower solid (green) line represents the HC terms. The combination of these corrections (TOT) is represented by the central (red) band including the uncertainties. The vertical line corresponds to $R=0.7$.

$$
6 \times \frac{1 \mathrm{GeV} \pm 1.2 \mathrm{GeV}}{P_{T}} \approx \frac{6 \mathrm{GeV}}{P_{T}} \pm \frac{7 \mathrm{GeV}}{P_{T}}
$$

Thus we estimate the fractional uncertainty from the underlying event and hadronization to be $7 \mathrm{GeV} / P_{T}$. We include this in the estimate of systematic theoretical errors by including a function $f_{7}\left(P_{T}\right)$ given by

$$
\begin{equation*}
f_{7}\left(P_{T}\right)=\frac{7 \mathrm{GeV}}{P_{T}} \tag{26}
\end{equation*}
$$

for LHC jets in the range $P_{T} \approx[100,1000] \mathrm{GeV}$.

## C. Summary: LHC

We now summarize the complete set of contributions to the uncertainty of the differential jet cross section as a function of $\left\{P_{T}, y\right\}$ for the LHC:


FIG. 11 (color online). Jet cross section $d^{2} \sigma / d P_{T} / d y$ vs $P_{T}$ in GeV with $y=0$ at the LHC $(\sqrt{s}=14 \mathrm{TeV})$ in units of $\mathrm{nb} / \mathrm{GeV}$. The line is a power law fit with $n=6$; this describes the slope of the jet data in the range $P_{T} \approx[100,1000] \mathrm{GeV}$.


FIG. 12 (color online). A compilation of the uncertainties for jet production at the $\operatorname{LHC}(\sqrt{s}=14,000 \mathrm{GeV})$ for $y=\{0,1,2\}$. The numeric label corresponds to the error components summarized in Eq. (27). The upper thick (red) line is the quadrature sum of the individual errors.
$f_{1}\left(P_{T}, y\right)=\frac{4.56 \times 10^{-2}}{\log \left(M(y) / P_{T}\right)}, \quad f_{2}\left(P_{T}, y\right)=\frac{1.24 \times 10^{-2} y^{2}}{\log \left(M(y) / P_{T}\right)}$
$f_{3}\left(P_{T}, y\right)=5.36 \times 10^{-2}, \quad f_{4}\left(P_{T}, y\right)=0.536 \times 10^{-2} y^{2}$,
$f_{5}\left(P_{T}, y\right)=1.07 \times 10^{-2} \log \left(\frac{15 P_{T}}{M(y)}\right)$,
$f_{6}\left(P_{T}, y\right)=0.214 \times 10^{-2} y^{2} \log \left(\frac{15 P_{T}}{M(y)}\right)$,
$f_{7}\left(P_{T}, y\right)=\frac{7 \mathrm{GeV}}{P_{T}}$.
We display these results in Fig. 12. In the central rapidity $(y \sim 0)$ region for $P_{T} \gtrsim 500 \mathrm{GeV}$ the perturbative uncertainties are dominant and slowly rise with increasing $P_{T}$, while for $P_{T} \lesssim 500 \mathrm{GeV}$ the nonperturbative uncertainties become increasingly important. For $y=2$, the transition $P_{T}$ is closer to 300 GeV than 500 GeV .

## VIII. CONCLUSIONS

As the LHC prepares to take data, it is important that we be able to determine whether a physics signal is consistent with the standard model. For example, if we observe a signal that is inconsistent with the standard model predic-
tion, but this inconsistency includes only experimental errors, we cannot claim this is "new physics" until we demonstrate it is also inconsistent including both experimental and theoretical errors. This paper provides a framework to quantitatively make such a determination in the case of jet physics. Similarly, this paper provides a framework to quantitatively fit parton distribution functions to Tevatron and LHC jet data, including estimated errors from the theory.

The framework that we provide involves functions $f_{J}\left(P_{T}, y\right)$ that represent independent contributions to the theory error. We note that other authors might estimate the errors differently and thus produce different functions $f_{J}\left(P_{T}, y\right)$. We hope that this will happen and that the merit of different choices will be debated.

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# Regularization, Renormalization, and Dimensional Analysis: Dimensional Regularization meets Freshman E8BM 

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#### Abstract

We illustrate the dimensional regularization technique using a simple problem from elementary electrostatics. We contrast this approach with the cutoff regularization approach, and demonstrate that dimensional regularization preserves the translational symmetry. We then introduce a Minimal Subtraction $(M S)$ and a Modified Minimal Subtraction $(\overline{M S})$ scheme to renormalize the result. Finally, we consider dimensional transmutation as encountered in the case of compact extra-dimensions.


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11.10.Gh Renormalization
11.10.Kk Field theories in dimensions other than four
11.15.-q Gauge field theories
11.30.-j Symmetry and conservation laws

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## I. DIMENSIONAL REGULARIZATION

## A. Introduction and Motivation

In 1999, Gerardus 't Hooft and Martinus J.G. Veltman received the Nobel Prize in Physics "for elucidating the quantum structure of electroweak interactions in physics." In particular, they demonstrated that the nonabelian electroweak theory could be consistently renormalized to yield unique and precise predictions.

A key ingredient for their demonstration was the development of the dimensional regularization technique.[1, 2, 3] That is, instead of working in precisely $D=4$ spacetime dimensions, they generalized the dimension to be a continuous variable so they could compute the theory in $\mathrm{D}=4.01$ or $\mathrm{D}=3.99$ dimensions. ${ }^{1}$

An important property of the dimensional regularization is that it respects gauge and Lorentz symmetries; ${ }^{2}$ this is in contrast to the other regularization schemes (e.g., cutoff schemes, etc.) which violate these symmetries. The symmetries of the electroweak theory play an critical role in determining the dynamics of the particles and their interactions. Because it respects these symmetries, dimensional regularization has become a essential tool for the calculation of field theories.

While dimensional regularization is an powerful and

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A. E and V in arbitrary dimensions

## VIII. Conclusions

## Acknowledgment

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Figure 1: a) A right triangle specified by angles $\{\theta, \phi\}$ and hypotenuse $c$. b) The same triangular area can be described by two similar triangles of hypotenuse $a$ and $b$.
elegant technique, most examples and applications of dimensional regularization are in the context of complex higher-order Quantum Field Theory (QFT) calculations involving gauge and Lorentz symmetries. However, the virtues of dimensional regularization can be exhibited without the "distractions" of the associated QFT complexities.

In the present paper, we will apply the dimensional regularization method to a problem from an elementary undergraduate physics course, namely the electric potential of an infinite line of charge. [5, 6] The example is simple enough for the undergraduate to understand, yet contains many of concepts we encounter in a true QFT calculation. We will contrast the symmetry-preserving dimensional regularization approach with a symmetryviolating cutoff approach.

Imagining a variable number of dimensions can be a productive exercise. To explain the weak nature of the gravitational force physicists have recently posited the existence of "Extra Dimensions." Having considered space-time dimensions in the neighborhood of $D=4$, we briefly contemplate wider excursions of $D=4,5,6, \ldots$ dimensions.

## II. DIMENSION ANALYSIS: THE PYTHAGOREAN THEOREM

To illustrate utility of dimensional regularization and dimensional analysis, we warm-up with a pre-example. Our goal will be to demonstrate the Pythagorean Theorem, and our method will be dimensional analysis.

We consider the right triangle displayed in Fig. 1ra). From the Angle-Side-Angle (ASA) theorem, this can be uniquely specified using the two angles $\{\theta, \phi\}$ and the hypotenuse $c$. We now construct a formula for the area of the triangle, $A_{c}$, using only these variables: $\{c, \theta, \phi\}$. Note that $c$ has dimensions of length, and $\{\theta, \phi\}$ are dimensionless. From dimensional analysis, the area of the triangle must have dimensions of length squared. As $c$ is
the only dimensional quantity, the formula for $A_{c}$ must be of the form:

$$
\begin{equation*}
A_{c}=c^{2} f(\theta, \phi) \tag{1}
\end{equation*}
$$

where $f(\theta, \phi)$ is an unknown dimensionless function. Note that $f(\theta, \phi)$ cannot depend on the length $c$ as this would spoil the dimensionless nature of $f(\theta, \phi)$.

We now observe that we can divide the original triangle of Fig. [1-a) into two similar triangles of hypotenuse $a$ and $b$ as displayed in Fig. (1-b). Again, using the ASA theorem, we can represent the area of these triangles, $A_{a}$ and $A_{b}$, in terms of the variables $\{a, \theta, \phi\}$ and $\{b, \theta, \phi\}$, respectively. Again from dimensional considerations, these areas must be proportional to $a^{2}$ and $b^{2}$; thus, we obtain:

$$
\begin{equation*}
A_{a}+A_{b}=a^{2} f(\theta, \phi)+b^{2} f(\theta, \phi) \tag{2}
\end{equation*}
$$

Because all three triangles are similar, their areas are described by the same $f(\theta, \phi)$. It is important to note that the function $f(\theta, \phi)$ is universal, dimensionless, and scale-invariant.

Finally, we use "conservation of area" to obtain our result. Specifically, since the area of the original triangle $A_{c}$ is equal to the sum of the combined $A_{a}$ and $A_{b}$,

$$
\begin{equation*}
A_{a}+A_{b}=A_{c} \tag{3}
\end{equation*}
$$

We can substitute Eqs. (1) and (2) to obtain our desired result:

$$
\begin{align*}
a^{2} f(\theta, \phi)+b^{2} f(\theta, \phi) & =c^{2} f(\theta, \phi) \\
a^{2}+b^{2} & =c^{2} \tag{4}
\end{align*}
$$

The last equation is, of course, the Pythagorean Theorem. Clearly, there are much simpler methods to prove this theorem; however, this method does illustrate the power of the dimensional analysis approach. ${ }^{3}$ Additionally, we gain a new perspective on the Pythagorean Theorem in this proof as it is linked to conservation of area.

There are instances, such as renormalizable field theory, where use of dimensional analysis tools are essential to making certain calculations tractable. The following example will illustrate some of these features.

## III. AN INFINITE LINE OF CHARGE

## A. Statement of the problem

For our next example we consider the calculation of the electric potential $V$ for the case of an infinite line of

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Figure 2: Coordinate system for an infinite line of charge running in the $y$-direction. We compute the potential $V(x)$ at a fixed perpendicular distance $x$ from the line of charge. The distance to the element of charge $d Q$ is $r=\sqrt{x^{2}+y^{2}}$.
charge with linear charge density $\lambda=Q / L$. The contribution to the electric potential from an infinitesimal charge $d Q$ is given by: ${ }^{4}$

$$
d V=\frac{1}{4 \pi \epsilon_{0}} \frac{d Q}{r}
$$

We choose our coordinate system (cf., Fig. (2) such that $x$ specifies the perpendicular distance from the wire, $y$ is the coordinate along the wire, and $r=\sqrt{x^{2}+y^{2}}$. Given $\lambda=Q / y$ we have $d Q=\lambda d y$ and can integrate along the length of the wire to obtain:

$$
\begin{equation*}
V(x)=\frac{\lambda}{4 \pi \epsilon_{0}} \int_{-\infty}^{+\infty} \frac{d y}{\sqrt{x^{2}+y^{2}}}=\infty \tag{5}
\end{equation*}
$$

Unfortunately, this integral is logarithmically divergent and a we obtain an infinite result.

## B. Scale invariance:

If we take a closer look at this integral, we will demonstrate that it is scale invariant; that is, if we rescale the argument $x$ by a constant factor $k,(x \rightarrow k x)$, the result is invariant.

$$
\begin{align*}
V(k x) & =\frac{\lambda}{4 \pi \epsilon_{0}} \int_{-\infty}^{+\infty} d y \frac{1}{\sqrt{(k x)^{2}+y^{2}}} \\
& =\frac{\lambda}{4 \pi \epsilon_{0}} \int_{-\infty}^{+\infty} d(y / k) \frac{1}{\sqrt{x^{2}+(y / k)^{2}}} \\
& =\frac{\lambda}{4 \pi \epsilon_{0}} \int_{-\infty}^{+\infty} d z \frac{1}{\sqrt{x^{2}+z^{2}}}  \tag{6}\\
& =V(x) \tag{7}
\end{align*}
$$

[^264]In the above we have implemented the rescaling $z=y / k$; since both $y$ and $z$ are dummy variables and the integration limits are infinite, the integral is unchanged. A consequence of this scale invariance is:

$$
\begin{equation*}
V\left(x_{1}\right)=V\left(x_{2}\right) \tag{8}
\end{equation*}
$$

At first glance, this result appears to be a disaster since the usual purpose of the electric potential is to compute the work $W$ via the formula

$$
W / Q=\Delta V=V\left(x_{2}\right)-V\left(x_{1}\right)
$$

or to compute the electric field via

$$
\vec{E}=-\vec{\nabla} V
$$

As Eq. (8) suggests $V\left(x_{2}\right)-V\left(x_{1}\right)=0$, this implies that our attempts to compute the work $W$ or the electric field $\vec{E}$ will be meaningless.

We now understand why it is fortunate that $V(x)$ is infinite as infinite numbers have some unusual properties. For example, for a finite constant $c$ we can write (schematically) $\infty+c=\infty$ which implies $\infty-\infty=c$. We now understand that even though we have $V\left(x_{1}\right)=$ $V\left(x_{2}\right)$, because these quantities are infinite we can still find that the difference is non-zero: $V\left(x_{2}\right)-V\left(x_{1}\right) \neq 0$. The challenge is that the difference of two infinite quantities is ambiguous; that is, how can tell if $\infty-\infty=c_{1}$ or $\infty-\infty=c_{2}$ is the correct physical result?

The solution is that we must regularize the infinite quantities so that we can uniquely extract the difference.

## IV. CUTOFF REGULARIZATION:

## A. Cutoff Regularization Computation

We will first regularize the integral using a simple cutoff method. That is, instead of considering an infinite wire, we will compute the potential for a finite wire of length $2 L$. In this instance, the potential becomes: ${ }^{5}$

$$
\begin{align*}
V(x) & =\frac{\lambda}{4 \pi \epsilon_{0}} \int_{-L}^{+L} d y \frac{1}{\sqrt{x^{2}+y^{2}}} \\
& =\frac{\lambda}{4 \pi \epsilon_{0}} \log \left[\frac{+L+\sqrt{L^{2}+x^{2}}}{-L+\sqrt{L^{2}+x^{2}}}\right] \tag{9}
\end{align*}
$$

We make the following observations.

- The result is finite.

[^265]- In addition to the physical length scale $x, V(x)$ depends on an artificial regulator $L$.
- We cannot remove the regulator $L$ without $V(x)$ becoming singular.
- The result for $V(x)$ violates a symmetry of the original problem-translation invariance.


## B. Computation of $E$ and $\delta V$

Even though $V(x)$ depends on the artificial regulator $L$, we observe that all physical quantities are independent of this regulator in the limit $L \rightarrow \infty$. Specifically, for the electric field we have:

$$
\begin{aligned}
E(x)= & \frac{-\partial V(x)}{\partial x}=\frac{\lambda}{2 \pi \epsilon_{0} x} \frac{L}{\sqrt{L^{2}+x^{2}}} \\
& \longrightarrow \frac{\lambda}{2 \pi \epsilon_{0} x}
\end{aligned}
$$

and for the potential difference (proportional to the electric work $W$ ) we have:

$$
\begin{equation*}
\delta V=V\left(x_{1}\right)-V\left(x_{2}\right) \longrightarrow \frac{\lambda}{L \rightarrow \infty} \log \left[\frac{x_{2}^{2}}{x_{1}^{2}}\right] \tag{10}
\end{equation*}
$$

## C. Broken translational symmetry:

Notice that the presence of the cutoff $L$ breaks the translation symmetry of the original problem. That is, for a truly infinite wire, our position in the $y$-direction is inconsequential; however, for a finite wire this is no longer the case. Specifically, if we shift our $y$-position by a constant $c$ to $y \rightarrow y^{\prime}=y+c$, our result becomes:

$$
\begin{align*}
V(x) & =\frac{\lambda}{4 \pi \epsilon_{0}} \int_{-L+c}^{+L+c} d y \frac{1}{\sqrt{x^{2}+y^{2}}}  \tag{11}\\
& =\frac{\lambda}{4 \pi \epsilon_{0}} \log \left[\frac{+(L+c)+\sqrt{(L+c)^{2}+x^{2}}}{-(L-c)+\sqrt{(L-c)^{2}+x^{2}}}\right]
\end{align*}
$$

Clearly we have lost the translation invariance $y \rightarrow y^{\prime}=$ $y+c$.

While preserving symmetries is not of paramount importance in this simple example, it is essential for certain field theory calculations. We now repeat the this calculation, but instead using dimensional regularization which will preserve the translational symmetry.

## D. Recap

In summary, we find that our problem is solved at the expense of 1 ) an extra scale $L$ which serves to both regu-

| $n$ | $\Omega(n)$ | $\Gamma(n / 2)$ |
| :---: | :---: | :---: |
| 1 | 2 | $\sqrt{\pi}$ |
| 2 | $2 \pi$ | 1 |
| 3 | $4 \pi$ | $\frac{\sqrt{\pi}}{2}$ |
| 4 | $2 \pi^{2}$ | 1 |

Table I: Angular integration measure as a function of dimension $n$. We recognize $\Omega(1)$ as the 1 -dimensional integration measure of $\int_{-1}^{+1} d r, \Omega(2)$ as the circumference of the unit circle, $\Omega(3)$ as the surface area of the unit sphere, and $\Omega(4)$ as the 3 -volume of the 4 -dimensional unit hypercube.
lates the infinities and provide an auxiliary length scale, and 2) a broken symmetry-translational invariance.

## V. DIMENSIONAL REGULARIZATION

## A. Generalization to arbitrary dimension

The central idea of dimensional regularization is to compute $V(x)$ in $n$-dimensions where $n$ is not necessarily an integer.[2, 3] We can generalize the integration of Eq. (5) by replacing the one-dimensional integration $d y=d^{1} y$ by the general $n$-dimension result:

$$
\begin{equation*}
d y \longrightarrow d^{n} y=\frac{d \Omega_{n}}{2} y^{n-1} d y \tag{12}
\end{equation*}
$$

where the angular integration measure is given by

$$
\begin{equation*}
\Omega_{n}=\int d \Omega_{n}=\frac{2 \pi^{n / 2}}{\Gamma\left(\frac{n}{2}\right)} \tag{13}
\end{equation*}
$$

It is instructive to verify that $\Omega_{n}$ yields the expected result for integer dimensions as tabulated in Table $\mathbb{I}$

## B. Computation of V in arbitrary dimensions

The generalized formula for $V(x)$ now reads: [6]

$$
\begin{equation*}
V(x)=\frac{\lambda}{4 \pi \epsilon_{0}} \int_{0}^{+\infty} d \Omega_{n} \frac{y^{n-1}}{\mu^{n-1}} \frac{d y}{\sqrt{x^{2}+y^{2}}} \tag{14}
\end{equation*}
$$

Note that we have introduced an auxiliary scale factor of $\mu^{n-1}$, where $\mu$ has units of length, to ensure $V(x)$ has the correct dimension. ${ }^{6}$ Replacing $n=1-2 \epsilon$ to facilitate expanding about $n=1$ we obtain

[^266]\[

$$
\begin{align*}
V(x) & =\frac{\lambda}{4 \pi \epsilon_{0}} \frac{\Gamma\left[\frac{1-n}{2}\right]}{\left(\frac{x}{\mu} \sqrt{\pi}\right)^{1-n}} \\
& =\frac{\lambda}{4 \pi \epsilon_{0}}\left(\frac{\mu^{2 \epsilon}}{x^{2 \epsilon}} \frac{\Gamma[\epsilon]}{\pi^{\epsilon}}\right) \tag{15}
\end{align*}
$$
\]

We make the following observations about the dimensionally regularized result.

- $V(x)$ depends on an artificial regulator $\epsilon$ which is dimensionless.
- $V(x)$ depends on an auxiliary scale $\mu$ which has dimensions of length.
- If we remove either the regulator $\epsilon$ or the auxiliary scale $\mu$ then $V(x)$ will become ill-defined.
- The dimensional regularization preserves the translation invariance of the original problem.

It is interesting to contrast this result with the cutoff regularization method where $L$ serves as both the regulator and the auxiliary scale.

## C. Computation of $E$ and $\delta V$

For the potential difference we find

$$
\begin{equation*}
\delta V=V\left(x_{1}\right)-V\left(x_{2}\right) \underset{\epsilon \rightarrow 0}{\longrightarrow} \frac{\lambda}{4 \pi \epsilon_{0}} \log \left[\frac{x_{2}^{2}}{x_{1}^{2}}\right] \tag{16}
\end{equation*}
$$

and for the electric field we obtain:

$$
\begin{align*}
E & =\frac{-\partial V(x)}{\partial x}=\frac{\lambda}{4 \pi \epsilon_{0}}\left[\frac{2 \epsilon \mu^{2 \epsilon} \Gamma[\epsilon]}{\left.\pi^{\epsilon} x^{1+2 \epsilon}\right]}\right. \\
\underset{\epsilon \rightarrow 0}{\longrightarrow} & \frac{\lambda}{2 \pi \epsilon_{0}} \frac{1}{x} \tag{17}
\end{align*}
$$

As before, we observe that all physical quantities are independent of both the regulator $\epsilon$ and the auxiliary scale $\mu$.

## D. The Renormalization Group Equation

The fact that the physical observables are independent of the un-physical auxiliary scale $\mu$ is simply a consequence of the renormalization group equation: ${ }^{7}$

$$
\begin{equation*}
\mu \frac{d \sigma}{d \mu}=0 \tag{18}
\end{equation*}
$$

[^267]where $\sigma$ represents any physical observable. Thus, the renormalization group equation implies that the electric field $\vec{E}=\vec{\nabla} V$ and the work $W=\delta V$ are also independent of the $\mu$ scale:
$$
\mu \frac{d E}{d \mu}=0 \quad \mu \frac{d W}{d \mu}=0
$$

These results are implicit in the final expressions for $E$ and $V$.

## E. Recap

In conclusion we find that the problem for $V(x)$ is solved at the expense of an artificial regulator $\epsilon$ and an auxiliary scale $\mu$. We also note the regulator $\epsilon$ and auxiliary scale $\mu$ are separate entities in contrast to the cutoff regularization method where the length $L$ plays both roles. Additionally, translational invariance symmetry is preserved; the fact that dimensional regularization respects symmetries makes this technique indispensable for field theory calculations involving gauge symmetries and Lorentz symmetries.

## VI. RENORMALIZATION

Having demonstrated two separate methods to regularize the infinities that enter the calculation of $V(x)$, we now turn to renormalization.

While physical quantities such as the work $W \sim \delta V$ and the electric field $\vec{E} \sim-\vec{\nabla} V$ are derived from $V(x)$, the potential itself is not a physical quantity. In particular, we can shift the potential by a constant $c, V \rightarrow V+c$, and the physical quantities will be unchanged.

To illustrate this point, let's expand $V(x)$ of Eq. (15) in powers of $\epsilon$ :

$$
V(x)=\frac{\lambda}{4 \pi \epsilon_{0}}\left[\frac{1}{\epsilon}+\ln \left[\frac{e^{-\gamma_{E}}}{\pi}\right]+\ln \left[\frac{\mu^{2}}{x^{2}}\right]+\mathcal{O}(\epsilon)\right]
$$

Let us now invent a Minimal Subtraction (MS) prescription. I have the freedom to shift $V(x)$ by a constant, and I design this to eliminate the $1 / \epsilon$ term:

$$
V_{M S}(x)=\frac{\lambda}{4 \pi \epsilon_{0}}\left[\ln \left[\frac{e^{-\gamma_{E}}}{\pi}\right]+\ln \left[\frac{\mu^{2}}{x^{2}}\right]+\mathcal{O}(\epsilon)\right]
$$

I can go even further and invent a Modified Minimal Subtraction $(\overline{M S})$ prescription to eliminate the $\ln \left[e^{-\gamma_{E}} / \pi\right]$ term as well:

$$
V_{\overline{M S}}(x)=\frac{\lambda}{4 \pi \epsilon_{0}}\left[\quad \ln \left[\frac{\mu^{2}}{x^{2}}\right]+\mathcal{O}(\epsilon)\right]
$$

After renormalization we can remove the regulator $(\epsilon \rightarrow$ 0 ), but not the auxiliary scale $\mu$; recall that without an
auxiliary scale to generate a dimensionless ratio $\mu / x$ we could not have any substantive $x$-dependence.

In addition to the $\mu$-dependence we will also have renormalization scheme dependence in $V(x)$. However, physical observables must be independent of the auxiliary scale $\mu$ and the particular renormalization scheme. For example, the computed potential differences yield identical results when calculated consistently in a single renormalization scheme:

$$
V_{M S}\left(x_{1}\right)-V_{M S}\left(x_{2}\right)=\delta V=V_{\overline{M S}}\left(x_{1}\right)-V_{\overline{M S}}\left(x_{2}\right)
$$

Here, the results of the Minimal Subtraction (MS) and the Modified Minimal Subtraction ( $\overline{M S}$ ) are identical for physical quantities.

However, if you mix renormalization schemes inconsistently you will obtain non-sensible results that are dependent on the choice of scheme: ${ }^{8}$

$$
V_{\overline{M S}}\left(x_{1}\right)-V_{M S}\left(x_{2}\right) \neq \delta V \neq V_{M S}\left(x_{1}\right)-V_{\overline{M S}}\left(x_{2}\right)
$$

## A. Connection to QFT

This elementary problem of the infinite line charge contains all the key concepts of the dimensional regularization and renormalization that we encounter in the full QFT radiative calculations. For example, in the radiative Quantum Chromodynamics (QCD) calculation of the Drell-Yan process ( $q \bar{q} \rightarrow \gamma^{*} \rightarrow \mu^{+} \mu^{-}$) we encounter the following infinite expression: ${ }^{9}$

$$
\begin{aligned}
\frac{D(\epsilon)}{\epsilon} & =\left(\frac{4 \pi \mu^{2}}{Q^{2}}\right)^{\epsilon} \frac{\Gamma(1-\epsilon)}{\Gamma(1-2 \epsilon)} \\
& \sim \frac{1}{\epsilon}-\ln \left(\frac{e^{+\gamma_{E}}}{4 \pi}\right)+\ln \left(\frac{\mu^{2}}{Q^{2}}\right)
\end{aligned}
$$

In this equation, $Q$ represents the characteristic energy scale; this is the independent variable that is analogous to $x$ in our example. While this is for a 4-dimensional QCD calculation, the structure of the divergent term is remarkably similar to our simple one-dimensional example above. For the QCD calculation, the Minimal Subtraction ( $M S$ ) prescription for this Drell-Yan calculation eliminates the $1 / \epsilon$ term, and the Modified Minimal Subtraction $(\overline{M S})$ prescription for this Drell-Yan calculation eliminates the $1 / \epsilon-\ln \left[e^{+\gamma_{e}} /(4 \pi)\right]$ so that only the $\ln \left[\mu^{2} / Q^{2}\right]$ remains.

[^268]| $D_{\text {eff }}$ | $E(r)$ | $V(r)$ | Example |
| :---: | :---: | :---: | :---: |
| 3 | $\frac{1}{r^{2}}$ | $\frac{1}{r}$ | Point charge |
| 2 | $\frac{1}{r^{1}}$ | $\ln r$ | Line charge |
| 1 | $\frac{1}{r^{0}}$ | $r$ | Sheet charge |

Table II: Example charge configurations that illustrate $D_{\text {eff }}=$ $\{3,2,1\}$ effective dimensions.

## VII. EXTRA DIMENSIONS

## A. E and V in arbitrary dimensions

In the above example, we used the mathematical trick of generalizing the number of integration dimensions from an integer to a continuous parameter. While we only let the dimension stray by $2 \epsilon$, it is useful to consider more drastic shifts as in the case of "Extra-Dimensions" which have recently been hypothesized.[11, 12] In this section, we provide an example of a dimensional transmutation; that is where the effective dimension $D_{\text {eff }}$ changes from one integer to another as we probe the system at different scales.

For example, we can generalize the $r$-dependence of the potential and electric field in for the case of $D$-dimensions as: ${ }^{10}$

$$
V(r) \sim \frac{1}{r^{D-2}} \quad E(r) \sim \frac{1}{r^{D-1}}
$$

A quick check will verify that this reproduces the usual expressions in ordinary $D=3$ spacial dimensions. Additionally, in 3-dimensions we can create charge distributions that mimic lower order spatial dimensions; this is illustrated in Table II For a (zero-dimensional) pointcharge in 3 -dimensions, according to Gauss's law the electric field lines spread out on a surface of $D-1=2$ dimensions, and we observe $E(r) \sim 1 / r^{2}$. Similarly, for a (onedimensional) line-charge, our space is now effectively $D=2$ dimensional; hence the electric field lines spread out on a surface of $D-1=1$ dimension, and we observe $E(r) \sim 1 / r$. Finally, for a (two-dimensional) sheetcharge, our space is now effectively $D=1$ dimensional; hence the electric field lines spread out on in $D-1=0$ dimensions, and we observe $E(r) \sim 1 / r^{0}=$ constant.

Figure 3 displays the electric field lines for a point charge confined to one infinite dimension $(x)$ and one finite (or compact) dimension ( $y$ ) of scale $R$. We observe that if we examine the electric field at scales small compared to the compact dimension $R(r \ll R)$, we find the the electric field lines spread out in 2 dimensions and we obtain the usual 2-dimensional result $\vec{E}(r) \sim 1 / r$; conversely, if we examine the electric field at distance scales

[^269]

Figure 3: Electric field for a point charge confined in one infinite dimension $(x)$ and one finite dimension $(y)$ of scale $R$.
large compared to the compact dimension $R(r \gg R)$, we find the 1-dimensional result $\vec{E}(r) \sim$ constant. In this example, the effective dimension of our space changes as we move from small $(D=2)$ to large length scales ( $D=1$ ).

## VIII. CONCLUSIONS

In this paper we have computed the potential of an infinite line of charge using dimensional regularization. By contrasting this calculation with the conventional cutoff
approach, we demonstrated that dimensional regularization respects the symmetries of the problem-namely, translational invariance. The dimensional regularization requires that we introduce a regulator $\epsilon$ and an auxiliary length scale $\mu$. We then renormalized the potential to eliminate the $1 / \epsilon$ singularities; this potential was finite and independent of the regulator $\epsilon$, but it depended on the particular renormalization scheme. However, we demonstrated that all physical observables $(E, \delta V)$ were scheme and scale invariant.

As this example exhibits many of the key features of dimensional regularization as applied to QFT, it provides an excellent opportunity to understand the virtues of this regularization method without the complications of gauge symmetries. As such, this example serves as an ideal pedagogical study.

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The EIC Science case: a report on the joint BNL/INT/JLab program

# Gluons and the quark sea at high energies: distributions, polarization, tomography 

Institute for Nuclear Theory, University of Washington, USA
September 13 to November 19, 2010

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## Foreword

The study of the fundamental structure of nuclear matter is a central thrust of physics research in the United States. As indicated in Frontiers of Nuclear Science, the 2007 Nuclear Science Advisory Committee long range plan, consideration of a future Electron-Ion Collider (EIC) is a priority and will likely be a significant focus of discussion at the next long range plan. We are therefore pleased to have supported the ten week program in fall 2010 at the Institute of Nuclear Theory which examined at length the science case for the EIC. This program was a major effort; it attracted the maximum allowable attendance over ten weeks.

This report summarizes the current understanding of the physics and articulates important open questions that can be addressed by an EIC. It converges towards a set of "golden" experiments that illustrate both the science reach and the technical demands on such a facility, and thereby establishes a firm ground from which to launch the next phase in preparation for the upcoming long range plan discussions. We thank all the participants in this productive program. In particular, we would like to acknowledge the leadership and dedication of the five co-organizers of the program who are also the co-editors of this report.

David Kaplan, Director, National Institute for Nuclear Theory
Hugh Montgomery, Director, Thomas Jefferson National Accelerator Facility
Steven Vigdor, Associate Lab Director, Brookhaven National Laboratory

## Preface

This volume is based on a ten-week program on "Gluons and the quark sea at high energies", which took place at the Institute for Nuclear Theory (INT) in Seattle from September 13 to November 19, 2010. The principal aim of the program was to develop and sharpen the science case for an Electron-Ion Collider (EIC), a facility that will be able to collide electrons and positrons with polarized protons and with light to heavy nuclei at high energies, offering unprecedented possibilities for in-depth studies of quantum chromodynamics. Guiding questions were

- What are the crucial science issues?
- How do they fit within the overall goals for nuclear physics?
- Why can't they be addressed adequately at existing facilities?
- Will they still be interesting in the 2020 's, when a suitable facility might be realized?

The program started with a five-day workshop on "Perturbative and Non-Perturbative Aspects of QCD at Collider Energies", which was followed by eight weeks of regular program and a concluding four-day workshop on "The Science Case for an EIC".

More than 120 theorists and experimentalists took part in the program over ten weeks. It was only possible to smoothly accommodate such a large number of participants because of the extraordinary efforts of the INT staff, to whom we extend our warm thanks and appreciation. We thank the INT Director, David Kaplan, for his strong support of the program and for covering a significant portion of the costs for printing this volume. We gratefully acknowledge additional financial support provided by BNL and JLab.

The program was structured along several subtopics, which roughly correspond to the chapters in this report. For each topic, convenors were appointed, who played an important role in the scientific organization of the program weeks and in editing the corresponding chapters. We gratefully thank them for their work. Special thanks are due to Matt Lamont and Marco Stratmann, who took on the lion's share in the painstaking task of merging the different chapters and making final edits.

Last but not least, we thank all participants of the INT program and all authors of this report for the work and enthusiasm they put into their contributions. Thanks to their efforts, much progress has been achieved, and we hope that the community will keep this momentum going in the continuing effort to build a compelling case for an Electron-Ion Collider.

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# Executive summary 

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## Introduction

Understanding the fundamental structure of matter in the physical universe is one of the central goals of scientific research. Strongly bound atomic nuclei predominantly constitute the matter from which humans and the observable physical world around us are formed. In the closing decades of the twentieth century, physicists developed a beautiful theory, Quantum Chromodynamics (QCD), which explains all strongly interacting matter in terms of point-like quarks interacting by the exchange of gauge bosons, known as gluons. Experiments have verified QCD quantitatively in processes involving a very large momentum exchange between the sub-atomic participants. Further confidence is obtained from significant progress in numerical computations of the static properties of the theory, in particular the excellent agreement of theory with the mass spectrum of low lying hadron resonances.

However, more than thirty years after QCD was first proposed as the fundamental theory of the strong force, and despite impressive theoretical and experimental progress made in the intervening decades, the understanding of how QCD works in detail remains an outstanding problem in physics. Very little is known about the dynamical basis of hadron structure in terms of the fundamental quark and gluon fields of the theory. How do these fundamental degrees of freedom dynamically generate the mass, spin, motion, and spatial distribution of color charges inside hadrons with varying momentum resolution and energy scales? Deep Inelastic Scattering (DIS) experiments at the HERA collider revealed clearly that at high momentum resolution and energy scales, the proton is a complex, many-body system of gluons and sea quarks, a picture very different from a more familiar view of the proton as a few point-like partons (a term that collectively refers to both quarks and gluons), each carrying a large fraction of its momentum. This picture, which is confirmed at hadron colliders, raises more questions than it answers about the dynamical structure of matter. For instance, how is the spin- $1 / 2$ of the proton distributed in this many-body system of sea quarks and gluons? In the early universe, how did the many-body plasma of quarks and gluons cool into hadrons with several simple structural properties? Recreating key features of this quark-hadron transition in heavy ion collisions has been a major activity in nuclear physics, with several surprising findings including the realization that this matter flows with very little resistance as a nearly perfect fluid. A deep understanding of the two cited examples, among many others, ultimately requires detailed knowledge of the quark-gluon structure of hadrons and nuclei.

This report on the science case for an Electron-Ion Collider (EIC) is the result of a ten-week program at the Institute for Nuclear Theory (INT) in Seattle (from September

13-November 19, 2010), motivated by the need to develop a strong case for the continued study of the QCD description of hadron structure in the coming decades. Hadron structure in the valence quark region will be studied extensively with the Jefferson Lab 12 GeV science program, the subject of an INT program the previous year. The focus of the INT program was on understanding the role of gluons and sea quarks, the important dynamical degrees of freedom describing hadron structure at high energies. Experimentally, the most direct and precise way to access the dynamical structure of hadrons and nuclei at high energies is with a high luminosity lepton probe in collider mode. An EIC with optimized detectors offers enormous potential as the next generation accelerator to address many of the most important, open questions about the fundamental structure of matter. The goal of the INT program, as captured in the writeups in this report, was to articulate these questions and to identify golden experiments that have the greatest potential to provide definitive answers to these questions.

At resolution scales where quarks and gluons become manifest as degrees of freedom, the structure of the nucleon and of nuclei is intimately connected with unique features of QCD dynamics, such as confinement and the self-coupling of gluons. Information on hadron sub-structure in DIS is obtained in the form of "snapshots" by the "lepton microscope" of the dynamical many-body hadron system, over different momentum resolutions and energy scales. These femtoscopic snapshots, at the simplest level, provide distribution functions which are extracted over the largest accessible kinematic range to assemble fundamental dynamical insight into hadron and nuclear sub-structure. For the proton, the EIC would be the brightest femtoscope scale lepton-collider ever, exceeding the intensity of the HERA collider a thousand fold. HERA, with its center-of-mass (CM) energy of 320 GeV , was built to search for quark substructure. An EIC, with its scientific focus on studying QCD in the regime where the sea quarks and gluons dominate, would have a lower CM energy. In a staged EIC design, the CM energy will range from $50-70 \mathrm{GeV}$ in stage I to approximately twice that for the full design. In addition to being the first lepton collider exploring the structure of polarized protons, an EIC will also be the first electron-nucleus collider, probing the gluon and sea quark structure of nuclei for the first time.

Following the same structure as the scientific discussions at the INT, this report is organized around the following four major themes:

- The spin and flavor structure of the proton
- Three dimensional structure of nucleons and nuclei in momentum and configuration space
- QCD matter in nuclei
- Electroweak physics and the search for physics beyond the Standard Model

In this executive summary, we will briefly outline the outstanding physics questions in these areas and the suite of measurements that are available with an EIC to address these. The status of accelerator and detector designs is addressed at the end of the summary. Tables of golden measurements for each of the key science areas outlined are presented on page 12 , In addition, each chapter in the report contains a comprehensive overview of the science topic addressed. Interested readers are encouraged to read these and the individual contributions for more details on the present status of EIC science.

## The spin and flavor structure of the proton

To understand how the constituents of the proton carry the proton's spin has been a defining question in hadron structure for several decades now. The proton spin problem presents the formidable challenge of understanding an essential feature of how a complex strongly-interacting many-body system organizes itself to produce a simple result. It goes directly to the heart of exploring and understanding the QCD dynamics of matter. From the surprising finding by the European Muon Collaboration that very little of the proton spin is provided by the spins of quarks and anti-quarks combined, the exploration of nucleon spin structure has by now developed into a world-wide quest central to nuclear and particle physics. To provide definitive answers in this area will be among the key tasks of an EIC.

Significant progress can be expected from the unique capability of an EIC to reach small momentum fractions $x$ and large momentum resolution scales $Q$, with high precision. A suite of measurements will be available. A golden measurement of nucleon spin structure at an EIC will be the precision study of the proton's spin structure function $g_{1}^{p}\left(x, Q^{2}\right)$ and its scaling violations, over wide ranges in $x$ and $Q^{2}$. As studies in this report will demonstrate, global analyses of spin-dependent parton distributions will determine the gluon helicity distribution $\Delta g$ and the quark singlet $\Delta \Sigma$ down to values of $x$ of about $10^{-4}$. This vastly extended reach should allow for the determination of the gluon and quark/anti-quark spin contributions to the proton spin to about $10 \%$ accuracy or better. The accuracy to which processes such as deeply-virtual Compton scattering can independently provide information on the remaining orbital angular momentum contributions will be addressed further in the section on spatial imaging.

An EIC will provide unprecedented insight into the flavor structure of the nucleon, a key element in mapping the "landscape" of hadron structure. There are two powerful golden measurements available at an EIC to achieve this. One of these methods, Semi-Inclusive Deep-Inelastic Scattering (SIDIS) has been used in previous fixed-target lepton scattering experiments HERMES and COMPASS. (Polarized proton-proton collisions at RHIC employ $W$-boson production for flavor identification.) At an EIC, semi-inclusive measurements would extend to much higher $Q^{2}$ than in fixed-target scattering, where the reaction becomes significantly cleaner, less contaminated with higher-twist effects (a technical term for contributions power suppressed in $1 / Q^{2}$ ), and therefore more tractable theoretically. The kinematic coverage for SIDIS in $x$ and $Q$ will be similar overall to what can be achieved in inclusive DIS. With the high luminosity of an EIC, extractions of the light-flavor helicity distributions $\Delta u, \Delta d$ and their anti-quark distributions from SIDIS will be possible with exquisite precision. With dedicated studies of kaon production, the strange and anti-strange distributions will also be accessible. All this will likely give insights into the question why it is that the combined quark and anti-quark spin contribution to the proton spin turns out to be so small.

The other independent method for accessing the quark and antiquark helicity distributions at an EIC is electroweak DIS. At high $Q^{2}$, the DIS process also proceeds significantly via the exchange of $Z$ and $W^{ \pm}$bosons. This gives rise to novel structure functions that are sensitive to various different combinations of the proton's helicity distributions. Studies show that both neutral current and charged current interactions would be observable at an EIC. To fully exploit the potential of an EIC for such measurements, positron beams are required, albeit not necessarily polarized. Besides the new insights into nucleon structure this would provide, studies of spin-dependent electroweak scattering at short distances with an EIC would be interesting physics in and of itself, much in the line of past and ongoing
electroweak measurements at HERA, Jefferson Lab, and RHIC.
Polarized electron-proton physics can be expected to take center stage at an EIC because these would be the first such collider measurements. However, as studies in this report show, there is a large potential for unpolarized physics at an EIC. Thanks to its high luminosity and the feasibility for an energy scan, an EIC would vastly improve upon HERA data on measurements of the longitudinal structure function $F_{L}$. This quantity is a key observable for studies of gluon structure and the possible transition to a high parton density or saturation regime in the proton. At an EIC, several SIDIS measurements of flavor distributions and multi-particle correlations will be possible for the first time. In particular, pinning down the strange quark and antiquark content of the proton would close one of the last notable gaps in our knowledge of unpolarized parton densities. Extended rapidity coverage will also allow for detailed studies of the rapidity gap structure of hard diffractive final states. In addition, the very high luminosities will bring a vast improvement in the precision of measurements of the charm and beauty contributions to nucleon structure.

## Three dimensional structure of hadrons and nuclei: Transverse momentum distributions

Partons can have a momentum component transverse to the direction of their parent nucleon and there exists experimental evidence to support an average transverse momentum of a few hundred $\mathrm{MeV} / \mathrm{c}$. However, much of our understanding of nucleon structure is in terms of integrated parton distributions that are only sensitive to the momentum resolution of the probe. A rigorous theoretical framework for parton transverse momentum distributions (TMDs) has been developed recently which allows for a description of specific scattering cross sections in terms of these distributions. TMDs are an essential step toward a more comprehensive understanding of the parton structure of the nucleon in QCD. An EIC will enable precise and detailed measurements of TMDs over a broad kinematic range.

For the scattering processes of interest, the large scale $Q^{2}$ justifies, in a leading twist approximation, the factorized description of the cross section in terms of several calculable or measurable factors, yielding a predictive framework. TMDs are examples of such measurable factors. In such descriptions not only does the magnitude of the parton transverse momentum enter, but also the transverse momentum direction, yielding strikingly asymmetric distributions. Several recently observed angular asymmetries are most naturally described by asymmetric, spin direction dependent TMDs.

A golden measurement at an EIC will be the Sivers asymmetry, a particular angular correlation between the target polarization and the direction of a produced final state hadron in polarized SIDIS. At the parton level, the Sivers effect is a spin-orbit coupling effect in QCD and is described by a TMD that quantifies how strongly the transverse momentum from orbital motion is coupled to spin. The Sivers effect is especially interesting because it is a consequence of phase interference peculiar to the gauge structure of QCD. The gauge invariant Sivers TMD is non-zero only if gluonic initial or final state interactions are taken into account. There is a calculable process dependence, most strikingly evident in SIDIS and Drell-Yan lepton pair production where the polarized Sivers function in the former is equal in magnitude but opposite in sign to the latter. Factorization breaking is also expected in more complicated processes, such as hadron-hadron collisions with hadronic final states. This process dependence has not yet been demonstrated but several such experiments, in particular at RHIC, will study the Sivers and other TMD effects. The comparison of these
results with complementary information from an EIC will allow a detailed understanding of the nature and extent of factorization breaking for TMDs.

A goal at an EIC is to obtain a flavor-separated extraction of the Sivers TMD in an energy regime where its theoretical interpretation is unambiguous. Percent level azimuthal asymmetries measured by HERMES, COMPASS and at Jefferson Lab at rather modest $Q^{2}$ have enabled rough first estimates of the magnitude of the Sivers effect. With the 12 GeV upgrade program at Jefferson Lab, the valence (large $x$ ) region will be explored in detail, whereas sea quark and gluon contributions at small $x$ (down to $10^{-4}$ ) will be mapped out with an EIC. The large $Q^{2}$ reach of an EIC will allow for extensive study of evolution effects in TMDs, and at large $x(x \sim 0.2)$ will have overlap with preceding experiments. High energies and high precision will enable a good understanding of the $x$ dependence of the Sivers functions for each quark flavor, including antiquarks and gluons. In addition, the larger transverse momentum range of final state particles at an EIC allows for studies of weighted asymmetries that are cleaner to interpret theoretically but are beyond the reach of fixed target experiments. The extensive transverse momentum range will for the first time in polarized SIDIS, allow studies of the transition region between the TMD description at low transverse momentum and the description in terms of collinear quark-gluon-quark correlation functions (known as the Qiu-Sterman mechanism) at high transverse momentum. Finally, with respect to previous SIDIS experiments and future Jefferson Lab experiments, a larger variety of final states can be considered at an EIC, such as (multiple) jets or Dmesons, all of great interest in isolating quark and gluon contributions to the various TMD effects.

Now that angular asymmetries consistent with the TMD framework have been observed, the road towards full-fledged experimental studies of TMDs can be mapped out and the essential role of an EIC identified. Besides the Sivers effect, essential information on the unpolarized TMD $f_{1}$ is obtained from unpolarized scattering cross sections. For reasons we shall outline, this extraction of $f_{1}$ can be classified as another golden measurement. This TMD determines the $Q^{2}$ dependence of the unpolarized cross section, which has been predicted but not yet verified. Predictions of the $x$, transverse momentum, scale and flavor dependence of $f_{1}$ allow for non-trivial checks of the fundamental TMD formalism corroborating and complementing what one learns from the Sivers and other spin TMD effects. The unpolarized SIDIS measurements at an EIC will give detailed information on the difference between sea and valence quark contributions, and on the role of gluons. Extracting unpolarized gluon TMDs at small $x$ is especially interesting because of the recently discovered agreement between predictions in the TMD framework and previous computations of the same in the Color Glass Condensate formalism as we shall discuss later.

The proposed silver experiments are 1) the distribution of transversely polarized quarks inside transversely polarized hadrons, 2) spin-orbit correlations inside unpolarized hadrons (the Boer-Mulders TMD), and 3) the Collins TMD fragmentation function, which describes a similar spin effect in the fragmentation of quarks into unpolarized hadrons. All three quantities involve transverse quark spin, which distinguishes them from the Sivers effect which deals with unpolarized partons inside a transversely polarized proton. An EIC will be able to provide multi-dimensional representations of all these quantities and the observables they give rise to. The TMD chapter illustrates by means of concrete examples and calculations how much further TMD studies can be pushed with an EIC compared to the present status. A prime example is shown in figure 2.11 on page 108 .

## Three dimensional structure of nucleons and nuclei: Spatial imaging

The high luminosity and large kinematic reach of an EIC offers unique possibilities for exploring the spatial distribution of sea quarks and gluons in the nucleon and in nuclei. The "imaging" of partons is possible in suitable exclusive reactions. The transverse position of the quark or gluon on which the scattering took place is obtained by a Fourier transform from the transverse momentum of the scattered nucleon or nucleus. At the same time, the longitudinal momentum loss of the target is correlated with the longitudinal momentum fraction $x$ of the parton. By choosing particular final states, measurements at an EIC will be able to selectively probe the spatial distribution of sea quarks and gluons in a wide range of $x$. Such 'tomographic images' will provide essential insight into QCD dynamics inside hadrons, such as the interplay between sea quarks and gluons, the role of pion degrees of freedom at large transverse distances and, from a more general perspective, the mechanism for confinement in QCD.

The quantities that encode this tomographic information are generalized parton distributions (GPDs). The formalism of GPDs is applicable in the full range of $x$. An alternative description at small $x$ is the dipole formalism, which is expressed in terms of the amplitude for small color dipoles to scatter off gluons in the hadron target. GPDs allow direct comparison of tomographic images for sea quarks and gluons with their counterparts in the valence quark region, where the 12 GeV program at Jefferson Lab will obtain information of unprecedented accuracy.

Potential golden measurements for parton imaging at an EIC are deeply virtual Compton scattering and photo- or electro-production of $J / \psi$ mesons. For Compton scattering, there are a large number of observables that can be calculated with high precision, whereas a unique advantage of $J / \psi$ production is its sensitivity to gluons. A suite of further reaction channels play the role of "silver measurements", which will provide complementary information and in particular help separate different quark flavors. Among those exclusive channels whose cross sections grow with energy, deeply virtual Compton scattering demands the highest luminosity. Simulations performed during the INT program indicate that precise and multi-differential measurements of this process can be envisaged with the projected EIC luminosity (see figures 3.34, 3.35 and 3.37 on pages 203, 204 and 207). Detailed studies including detector effects will be required to establish the achievable experimental accuracy.

The envisaged configuration of an EIC interaction region and detector will provide data in a wide enough range of transverse momentum transfer to permit a Fourier analysis of observables. With this, exclusive cross sections and angular or polarization asymmetries will give direct quantitative information about the spatial distribution of partons in a specified range of $x$. Estimates indicate that transverse distances ranging from about 0.1 fm to 2 fm or higher will be accessible, provided that a good enough momentum resolution can be achieved experimentally. Such data will provide the basis for reconstructing generalized parton distributions and, ultimately, the joint distribution of partons in transverse position $b$ and longitudinal momentum fraction $x$. For this second step, an EIC's large lever arm in photon virtuality $Q^{2}$ at a given photon energy will be essential, since it is the scale evolution in $Q^{2}$ that carries the most detailed information about the longitudinal parton momentum.

Our current knowledge about the helicity distributions of quarks and gluons indeed suggests that the orbital angular momentum of partons plays a prominent role in the nucleon. Exclusive scattering on a transversely polarized target gives access to this degree of freedom
in parton tomography and allows one to study spin-orbit correlations at the parton level. An especially interesting aspect is the relation between a polarization induced asymmetry in transverse parton position and the Sivers asymmetry in transverse parton momentum. Such a relation is profoundly dynamical, and its quantitative exploration in the sea quark and gluon domain will be a highlight of exploring hadron structure and dynamics at an EIC. Deeply virtual Compton scattering will again play an essential role in this context, along with vector meson production channels. Quantitative estimates of the achievable statistical and systematic accuracy were not made during the INT program, but the necessary tools are now in place and results should be available soon.

Ji's angular momentum sum rule condenses the connection between generalized parton distributions and parton angular momentum into a single number for each quark flavor and for the gluon. To evaluate this sum rule from exclusive measurements is truly challenging for several reasons. The most serious among them is that one needs to reconstruct the full $x$ dependence of GPDs from observed scaling violations in $Q^{2}$. As already mentioned, the large kinematic coverage of an EIC provides a good starting point for such a program, but it remains to be seen which accuracy can be attained for the angular momentum. We regard this as a long-term endeavor, which will profit from the progress one can expect in the coming years from the 12 GeV program at Jefferson Lab.

## Physics opportunities in electron-nucleus collisions

An EIC would be the world's first $\mathrm{e}+\mathrm{A}$ collider. It will significantly extend parton studies of nuclear structure into the regime dominated by sea quarks and gluons. Prior fixed target DIS measurements on nuclei revealed that the ratio of nuclear to nucleon cross sections is significantly less than unity (normalized by the atomic mass number) both at large $x$ (the EMC effect) and at small $x$ (shadowing). These interesting nuclear phenomena were however only observed for valence and (to a lesser extent) sea quarks. The nuclear gluon distribution is very poorly constrained at all $x$ values, especially at $x<0.01$ where it is completely unknown. An EIC could reveal surprises in our fundamental understanding of the parton structure of nuclei in this terra incognita.

A fundamental feature of QCD is gluon saturation, which arises as a consequence of the fact that gluon distributions at a fixed $Q^{2}$ cannot grow rapidly indefinitely with decreasing $x$. The properties of matter in this novel saturation regime of strong color fields in QCD is described by a saturation scale which grows both with decreasing $x$ and with increasing nuclear size. Model estimates of this nuclear "oomph" give a saturation scale in a large nucleus at EIC energies to be of the same magnitude as the saturation scale in a proton at a TeV scale electron-proton collider; electron-nucleus collisions therefore provide an efficient method to explore saturation in QCD.

As a consequence of asymptotic freedom, the large saturation scale (relative to the intrinsic QCD scale $\Lambda_{Q C D}$ ) accessible at an electron-nucleus collider implies that the properties of saturated gluon matter at small $x$ can be computed systematically using weak coupling techniques and compared to experimental data. One such weak coupling approach is the Color Glass Condensate (CGC). Renormalization group (RG) methods in the CGC are used to compute observables in electron-nucleus collisions that are sensitive to the energy evolution of particular many-body gluon correlators. These correlators, classified as "dipole", "quadrupole" and "multipole" effective degrees of freedom from their color structure, are universal. Final states in proton-nucleus and nucleus-nucleus collisions can also
be expressed in terms of these objects. Properties of multipole degrees of freedom can be inferred from measurements of cross-sections for specific final states in one of these reactions and used as input in computations of cross-sections for other final states, thereby providing an important test of the validity and limits of the CGC effective theory. A further interesting possibility is that multipole correlators at very high energies become independent of the initial conditions specific to a particular nucleus that are inputs at a given $x$ scale to the RG evolution equations. While it appears unlikely that an EIC would have sufficient energy to access this asymptotic regime, DIS off different nuclei can provide important constraints on pre-asymptotic trends in that direction.

At large $x$ in nuclei, DIS corresponds to the virtual photon scattering off quarks, with the nucleus acting as an extended colored medium that interacts with the hard colored probe. Because the energy and momentum resolution of the probe can be accurately controlled in DIS, one can quantitatively address, with a precision unmatched at hadron colliders, interesting questions about the nature of multiple scattering and $p_{\perp}$ broadening, energy loss and fragmentation, and the propagation of heavy quarks and jets in colored media. Perturbatively calculable short distance physics can be isolated from the hadronization mechanism by tuning the energy and momentum resolution of the virtual photon probe to shed new light on the latter both in medium and in the vacuum. While some such studies have been performed previously at fixed target DIS facilities and in proton-nucleus collisions, the extended kinematic reach, collider geometry and precision probes will vastly add to their scope, allowing for definitive answers to enduring questions about in-medium properties of QCD. For instance, the propagation of heavy charm and beauty quarks in medium will be quantitatively studied in DIS for the first time. In addition to being interesting in their own right, DIS studies of parton propagation in "cold" QCD media are an important benchmark for a quantitative understanding of their role in the hot QCD medium produced at RHIC and the LHC.

An important opportunity to understand the role of gluons in the structure of short range nuclear forces is made possible by exclusive measurements with an EIC of open heavy flavor and quarkonium in DIS off light nuclei. Other interesting studies at large $x$ where the kinematic reach of an EIC will complement the Jefferson Lab 12 GeV program, including the EMC effect and generalized parton distributions for nuclei.

A number of experimental observables have been identified that can shed light on the compelling physics issues outlined. One set of golden measurements include the inclusive structure functions $F_{2}$ and $F_{L}$ for light and heavy nuclei. They will provide the first ever unambiguous measurements of nuclear gluon distributions. Studies of the evolution of quark singlet and gluon distributions with $x$ and $Q^{2}$ for light and heavy nuclei can systematically uncover the breakdown of leading twist evolution, the onset and development of non-linear saturation dynamics and enable the extraction of the corresponding saturation scale. Another set of golden measurements are provided by semi-inclusive DIS (SIDIS) off nuclei. Di-hadron correlations in particular, are very sensitive to non-linear QCD evolution, and allow for a clean extraction of the saturation scale. They will corroborate (or invalidate) claims of saturation seen in di-hadron correlations in deuteron-gold collisions; more generally, they enable the previously discussed tests of universality of multipole correlators at small $x$. Golden measurements at large $x$ are semi-inclusive production of light and heavy flavors and jets. These provide unique insight into energy loss and parton shower development in an extended colored medium, as well as into the dynamics of hadronization in this many-body environment. The heavy flavor and jet measurements will be the first of their kind in nuclear DIS; we note that feasibility studies for them are still in a preliminary stage.

In addition to these golden measurements, there are several important measurements classified as "silver" instead of gold only in a relative sense. The most important among these are the diffractive structure functions $F_{2, D}$ and $F_{L, D}$ which will be extracted for nuclei for the very first time. At HERA, these structure functions for protons constituted more than $15 \%$ of the cross-section; the predictions of saturation models is that this fraction will be significantly larger in nuclei. Exclusive production of vector mesons and deeply virtual Compton scattering probe the spatial distribution of partons in nuclei; at small $x$, they can help clarify the interplay between saturation and the effects of chiral symmetry breaking and confinement.

Finally, a frequently posed question is whether proton/deuteron-nucleus scattering can provide the same information content as electron-nucleus collisions. In the former, the computation of final states, in leading twist kinematics, contains convolutions over parton distributions in the nucleon projectile as well as that in the target. In addition, for a number of final states, a large number of parton scattering reactions are likely to contribute. This significantly compromises the accuracy to which one determines the parton structure of the target. For fundamental questions regarding the spatial distribution of partons and color singlet structures exchanged in hard diffractive scattering, there are essential qualitative differences in hadron-hadron and lepton-hadron processes arising from the lack of universality in key aspects of the dynamical structure of nucleons and nuclei. Thus while proton/deuteron-nucleus scattering at high energies has the strong potential to be a discovery machine for new QCD physics, uncovering the origins of such physics and its implications for our fundamental understanding of the parton structure of nuclei, will require an EIC.

## Electroweak interactions and physics beyond the Standard Model

While the physics of an EIC is primarily motivated by the study of strong interactions, its physics case is strengthened by its potential to contribute to electroweak studies as well. Experience has shown that a new accelerator that pushes the frontiers either in energy, and/or luminosity and intensity, is of interest for studies of electroweak physics. We have already mentioned that precision studies of (parity-violating) electroweak spin structure functions would be possible at an EIC, giving new insights into nucleon spin structure. However, the electroweak physics case for an EIC is broader as it would also allow measurements of parameters of electroweak theory. Studies presented in detail in the INT report suggest that for high energy and luminosity, there would be excellent prospects for extractions of the Weinberg angle, which should even be possible over a fairly wide range in $Q^{2}$ so that its running can be further studied in detail. In this way, an EIC would complement the precise LEP and SLD measurements on the $Z$-pole, atomic parity-violation measurements, the SLAC E158 Møller scattering data, and the NuTeV data whose final value is in fact around three standard deviations above the SM prediction. A comparison of EIC results for $\sin ^{2} \theta_{W}$ with those on the $Z$-pole in particular can be used to search for new physics effects. Some of the experimental systematics involved at an EIC are broadly understood, but may still need further work to clarify. A full "global survey" of electroweak parameters from EIC data - much in the spirit of the approach also taken at HERA - is still outstanding but planned. In addition, an EIC might possibly be able to open a direct window on beyond-Standard Model physics, assuming that conditions are favorable. Studies
indicate that the EIC might be able to perform a sensitive search for a third generation leptoquark in electron-tau conversion $e p \rightarrow \tau X$, with potential reach well beyond that in previous studies at HERA.

## EIC Accelerator Design

Two substantial, focused efforts at developing a design for an electron-ion collider in the U.S. based on existing accelerators are underway at Brookhaven National Laboratory and Thomas Jefferson National Accelerator Facility. At BNL, the eRHIC design utilizes a new linear electron accelerator to collide with the existing polarized proton and ion beams of the operating Relativistic Heavy Ion Collider (RHIC). At JLab, the ELIC design employs new electron and ion storage rings together with the 12 GeV upgraded existing CEBAF. Although based on two different, existing accelerators, because they are driven by the same science objectives, the two U.S. EIC design efforts have similar characteristics. The most important include:

- highly polarized (>70\%) electron and nucleon beams
- ion beams from deuterium to the heaviest nuclei - uranium or lead
- center of mass energies: from about 20 GeV to about 150 GeV
- maximum collision luminosity $\sim 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$
- non-zero crossing angle of colliding beams without loss of luminosity (so-called crab crossing)
- cooling of the proton and ion beams to obtain high luminosity
- staged designs where the first stage would reach CM energies of about 70 GeV
- the possibility to have multiple interaction regions

It is clear from the EIC physics studies that with a luminosity of $\sim 10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$, and operating for about a decade, ground breaking new experiments to probe our understanding of QCD will become feasible. This would require delivery of order $50 \mathrm{fb}^{-1}$ with polarized nucleon and heavy ion beams to experiments in about a decade. This would be 100 times more integrated luminosity than recorded over a decade at the only previous electron-proton collider, HERA at DESY. With a luminosity of $\sim 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$, precision imaging and electroweak experiments become feasible at an EIC.

The EIC accelerator designs being considered will require significant R\&D for realization. The cooling of the hadron beam is essential to attain the luminosities demanded by the science. The development of a new technique, coherent electron cooling, is underway at BNL while conventional electron cooling is being pushed to high RF power at JLab. Energy recovery linear accelerators at high energy and intensity are a key technology for an EIC. Further, the eRHIC design demands an increase in the intensity produced by polarized electron sources of over an order of magnitude beyond what is available at present. The ELIC design utilizes novel figure-8 storage rings for both electrons and ions.

In Europe, two electron-ion collider accelerators are under consideration. At the Large Hadron Collider at CERN, physicists are considering colliding an electron beam (either a
linac or ring) with an energy of about 70 GeV with the existing unpolarized proton and heavy-ion beams. The present LHeC design can reach a CM energy of about 1.4 TeV with a luminosity of $10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. At GSI in Germany, an Electron-Nucleon Collider (ENC) would be realized by colliding electrons in a 3 GeV storage ring with 15 GeV protons in the High Energy Storage Ring of the planned Facility for Antiproton and Ion Research (FAIR). The CM energy at an ENC is about 14 GeV and the expected luminosity is about $10^{32}$ $\mathrm{cm}^{-2} \mathrm{~s}^{-1}$. Thus, the two European colliders differ in CM energy by about two orders of magnitude, in colliding luminosity by about one order of magnitude, and have very different scientific objectives.

## EIC Detectors

Optimized detectors are essential to carry out the ground breaking experiments planned at an EIC. The design of EIC detectors is intimately connected to the design of the accelerator interaction regions (IR) through the location of magnets, configuration of crossing angles, and available space. A particular challenge is to detect forward-going scattered protons from exclusive reactions, as well as decay neutrons from the break-up of ions in incoherent diffraction. Past experience at colliders with lepton beams has shown that synchrotron radiation generated by bending the electron beam close to the IR can produce challenging backgrounds for detectors.

Detector concepts for an EIC are being developed and are guided both by the demands of the scientific program and by the experience with ZEUS and H1 at HERA. The EIC detector will certainly include a large central detector likely containing a solenoidal magnetic field (of order 4 T ); trackers for momentum and angular resolution; electromagnetic and hadronic calorimetry; particle identification involving Cerenkov detectors, and vertex detectors. Further, detectors in the forward and backward directions will be required to augment the large central detector. These are necessary to detect hadrons from low $x$ processes and will require particle identification, calorimetry (both electron and hadron) and possibly magnetic field. With multiple interaction regions, it may be more advantageous to consider different detectors (e.g. forward/backward vs. central, high luminosity vs. low luminosity) for different IRs.

Minimizing the effects of systematic uncertainties is an important aspect of detector design. Absolute and relative luminosity determination is a key to extracting important observables, for instance the longitudinal structure function or small polarization asymmetries. Measurement of the polarization of electron and hadron beams has a high priority. As with the accelerator, R\&D for EIC detectors will be essential.

## Tables of golden measurements

| Spin and flavor structure of the nucleon |  |  |  |
| :---: | :---: | :---: | :---: |
| Deliverables | Observables | What we learn | Requirements |
| polarized gluon | scaling violations | gluon contribution | coverage down to $x \simeq 10^{-4} ;$ |
| distribution $\Delta g$ | in inclusive DIS | to proton spin | $\mathcal{L}$ of about $10 \mathrm{fb}^{-1}$ |
| polarized quark and <br> antiquark densities | semi-incl. DIS for <br> pions and kaons | quark contr. to proton spin; <br> asym. like $\Delta \bar{u}-\Delta \bar{d} ; \Delta s$ | similar to DIS; |
| good particle ID |  |  |  |
| novel electroweak | inclusive DIS | flavor separation | $\sqrt{s} \geq 100 \mathrm{GeV} ; \mathcal{L} \geq 10 \mathrm{fb}^{-1}$ |
| spin structure functions | at high $Q^{2}$ | at medium $x$ and large $Q^{2}$ | positrons; polarized ${ }^{3} \mathrm{He}$ beam |


| Three-dimensional structure of the nucleon and nuclei: transverse momentum dependence |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Deliverables | Observables | What we learn | Phase I | Phase II |  |
| Sivers and | SIDIS with transv. | quantum interference | valence+sea | 3D Imaging of |  |
| unpolarized | polarization/ions; | multi-parton and | quarks, overlap | quarks and gluon; |  |
| TMDs for | di-hadron (di-jet) | spin-orbit | with fixed target | $Q^{2}\left(P_{\perp}\right)$ range |  |
| quarks and gluon | heavy flavors | correlations | experiments | QCD dynamics |  |


| Three-dimensional structure of the nucleon and nuclei: spatial imaging |  |  |  |
| :---: | :---: | :---: | :---: |
| Deliverables | Observables | What we learn | Requirements |
| sea quark and | DVCS and $J / \psi, \rho, \phi$ |  |  |
| gluon GPDs | transverse images of <br> production cross sect. <br> and asymmetries <br> sea quarks and gluons <br> in nucleon and nuclei; <br> total angular momentum; <br> onset of saturation | $\mathcal{L} \geq 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$, <br> Roman Pots <br> wide range of $x_{B}$ and $Q^{2}$ <br> $e^{+}$beam for DVCS $e^{-}$and $p$ beams |  |


| QCD matter in nuclei |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Deliverables | Observables | What we learn | Phase I | Phase II |  |
| integrated gluon | $F_{2, L}$ | nuclear wave function; <br> saturation, $Q_{s}$ | gluons at <br> $10^{-3} \leq x \leq 1$ | explore sat. <br> regime |  |
| $k_{T}$-dep. gluons; <br> gluon correlations | di-hadron <br> correlations | non-linear QCD <br> evolution/universality | onset of <br> saturation; $Q_{s}$ | RG evolution |  |
| transp. coefficients <br> in cold matter | large- $x$ SIDIS; <br> jets | parton energy loss, <br> shower evolution; <br> energy loss mech. | light flavors, charm <br> bottom; jets | precision rare <br> probes; <br> large- $x$ gluons |  |


| Electroweak interactions and physics beyond the Standard Model |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Deliverables | Observables | What we learn | Phase I | Phase II |  |
| Weak mixing | Parity violating |  |  |  |  |
| angle |  |  |  |  |  |
| asymmetries in |  |  |  |  |  |
| $e p$ - and $e d$-DIS |  |  |  |  |  | \(\left.\begin{array}{c}physics behind electroweak <br>

symmetry breaking <br>
and BSM physics\end{array} \quad $$
\begin{array}{c}\text { good precision } \\
\text { over limited } \\
\text { range of scales }\end{array}
$$ $$
\begin{array}{c}\text { high precision } \\
\text { over wide range } \\
\text { of scales }\end{array}
$$\right]\)

## Chapter 1

## The spin and flavor structure of the proton

Convenor and chapter editor:
M. Stratmann

### 1.1 Introduction and chapter overview

Marco Stratmann

Two weeks of the INT program on "Gluons and the Quark Sea at High Energies" were devoted to the physics of unpolarized and polarized parton distribution functions. A compelling set of physics opportunities at an EIC has emerged from lively discussions among the participants and subsequent interactions with the hadron structure community. This Chapter outlines the identified open fundamental questions in hadronic physics and the "golden measurements" and experimental requirements to thoroughly address them at a future EIC. The anticipated results will have a profound influence on our understanding of the spin and flavor structure of nucleons.

Sixteen years of operations at DESY-HERA had a transformational impact on the way we view the internal partonic content of nucleons and have led to various new developments in the field of Quantum Chromodynamics. The experiments have left a rich legacy of results, the most prominent ones being the strong rise of the gluon density at small momentum fractions $x$, the large portion of diffractive events, and the transition from high to low momentum transfer $Q$ for various processes. Likewise, vigorous experimental programs with polarized beams and targets in the past twenty-five years at all major laboratories have brought us closer to pinpoint the various contributions to the proton's spin. They also revealed novel, often puzzling phenomena which initiated new directions of research in spin physics such as transverse-momentum dependent parton densities; see Chapter 2.

In each case, the experimental progress was matched by considerable theoretical efforts in Quantum Chromodynamics. Most notable in this context are the level of precision reached in higher-order calculations in perturbative QCD and the much refined global analysis tools to reliably extract information on parton densities from data and to determine their uncertainties. Yet, there is still a significant lack of understanding on quite a few outstanding issues. An EIC will prove crucial in addressing them by making use of the anticipated high luminosities and the variability of beam energies.

Of course, due to the lower center-of-mass system energies of an EIC as compared to HERA one cannot extend the kinematic reach towards smaller values of $x$ for unpolarized electron-proton collisions. Also, over the next couple of years the CERN-LHC will provide a great deal of information on helicity-averaged parton densities in a broad range of $x$ from various different hard scattering processes up to very large resolution scales $Q$. The 12 GeV upgrade of the CEBAF facility at Jefferson Laboratory is designed to map parton distributions up to very large values of $x$ at scales $Q$ of a few GeV to test how well, for instance, counting rules apply. Therefore, we expect that most aspects of unpolarized parton densities will be sufficiently well known by the time an EIC is expected to turn on, with some important exceptions to be discussed below.

The situation is rather different for spin physics where the bulk of experimental information stems from fixed-target lepton-nucleon scattering experiments at rather low energies. Ideas to turn HERA into a polarized electron-proton collider never materialized. Existing experiments studying the helicity structure of the nucleon, like PHENIX and STAR at RHIC, will continue to add data in the next couple of years. In particular, measurements of double-spin asymmetries for di-jets in $p p$ collisions at 500 GeV should improve the current constraints on the polarized gluon density $\Delta g(x)$ and extend the covered $x$ range towards somewhat smaller values. Parity-violating, single-spin asymmetries for $W$ boson production should reach a level where they help to constrain the spin-dependent $u$ and $d$
quark and antiquark densities at medium-to-large $x$. At JLab-12 the focus is again on the large $x$ frontier at moderate values of $Q$ to address to what extent quarks obey helicity retention which predicts that in the limit $x \rightarrow 1$ quark and nucleon spins become fully aligned. Ultimately, all these efforts are limited by their kinematic coverage both in $x$ and in $Q$. Since the most fundamental open questions in spin physics concern the polarization of wee partons, see below, there are many opportunities for a high-energy polarized EIC to contribute significantly due to its unique capabilities to access values of $x$ down to about $10^{-4}$. This is central to finally determine and understand the role of quarks and gluons in the spin decomposition of the nucleon.

Factorization of experimental observables into non-perturbative parton densities and calculable hard scattering cross sections is the cornerstone for the theoretical application of QCD at high energies within perturbative methods. Available QCD calculations for inclusive and semi-inclusive deep-inelastic scattering processes will allow us to confront future high-statistics EIC data with theory at the necessary very high level of precision. A brief account of the status of perturbative QCD calculations for most of the key measurements at an EIC is given in Sec. 1.2.

Since the EIC is a natural extension of the physics program carried out at HERA both in terms of the anticipated significant increase in luminosity and the possibility to have polarized beams, we summarize the latest status of HERA data based on the recent combination of results from the H1 and ZEUS experiments in Sec. 1.3. This discussion also helps to expose the open questions about the structure of unpolarized nucleons an EIC can elucidate and which cannot be answered solely by measurements at the LHC. The most compelling ones comprise

- the longitudinal structure function $F_{L}$,
- the elusive strangeness and anti-strangeness densities,
- and heavy flavor contributions to deep-inelastic scattering.

A detailed account, including other second tier opportunities is given in Sec. 1.4.
An EIC could make the first precise measurement of $F_{L}$ in a kinematic range that overlaps both previous fixed-target and HERA data, none of which are very precise. $F_{L}$ is particularly sensitive to the gluon distribution and QCD dynamics at small $x$ which makes it a promising candidate to study the transition to the high parton density regime, i.e., the phenomenon of saturation, with an inclusive observable. While one does not expect non-linear effects to be of significant relevance in electron-proton collisions at an EIC, a measurement of $F_{L}$ provides the baseline for similar studies in electron-heavy ion collisions. Here, the onset of saturation effects is expected already at $x \simeq 10^{-3}$ which elevates $F_{L}$ to one of the golden measurements to be performed at the EIC; see Chapter 5 on QCD matter under extreme conditions for details. The determination of $F_{L}$ relies on an accurate measurement of the variation of the so-called reduced cross section for fixed values of $x$ and $Q$ at different c.m.s. energies $\sqrt{s}$. The large variability of beam energies at sustained large luminosities is a particular strength of an EIC and proves critical for this measurement. A first feasibility study for electron-proton collisions can be found in Sec. 1.6.

Semi-inclusive deep-inelastic production of identified pions and kaons is expected to be the most viable and promising way to determine differences among parton distribution functions for different quark flavors or between quarks and anti-quarks. Such measurements make use of the different probabilities for producing a certain hadron species from a given
quark flavor or gluon and have been successfully performed at fixed-target experiments such as HERMES. The EIC offers unprecedented opportunities to extend the kinematic reach toward small $x$ or large $Q$. In particular, the elusive strangeness density and a possible asymmetry between strangeness and anti-strangeness distributions can be deduced from charged kaon production yields. Prerequisites are excellent particle identification in most of the phase space and a thorough theoretical understanding of the hadronization of quarks and gluons into the observed hadrons. In collinear factorization, the latter information is encoded in non-perturbative fragmentation functions which are constrained by a wealth of available experimental data on single-inclusive hadron yields. Further significant progress on the quality of such fits is expected once upcoming data from $B$ factories and the LHC are included. In Sec. 1.5 we present a first feasibility study for charged kaon production at the EIC.

Heavy flavors, in particular charm quarks, can give a sizable contribution to deepinelastic scattering structure functions. Within the foreseen EIC kinematics, charm yields up to $10 \div 15 \%$ of the inclusive cross section. The theoretical framework for heavy quark production is much more complex than for light (massless) quarks due to the presence of multiple scales. The mass of the heavy quarks prevents them from having a partonic interpretation, and they can be only produced externally, for instance, by photon-gluon fusion. This framework yields a very good description of all available HERA data within the present uncertainties and is expected to be relevant also in the entire kinematic regime of an EIC. Nonetheless, one may introduce heavy quark densities for asymptotically large scales, i.e., $Q \gg m$, and smooth interpolation schemes have been devised which incorporate the correct threshold and asymptotic behavior. The relevant theoretical framework and recent progress on higher order calculations is briefly reviewed in Sec. 1.7.

The charm contribution to the longitudinal structure function $F_{L}$ is expected to be particularly sensitive to mass effects and has never been measured before. A first feasibility study within the kinematics of an EIC can be found in Sec.1.8. An EIC is also well suited to address the long-standing question of a possible relevance of a non-perturbative "intrinsic" charm contribution in the nucleon wave-function, mainly concentrated at large momentum fractions. Quantitative estimates based on models for an intrinsic charm contribution are promising and can be found in Sec. 1.9 ,

The physics opportunities with polarized lepton and proton beams are even more multifaceted and will address some of the most fundamental open questions in hadronic physics for which one has been seeking answers for more the two decades now. Thus, the anticipated results will have far-reaching impact on our understanding of the nucleon's spin structure. The unique capability of the EIC to reach small momentum fractions $x$ or large scales $Q$ in longitudinally polarized electron-proton collisions with high luminosity will enable us to explore in detail

- the polarized gluon distribution and its contribution to the proton's spin,
- the individual light quark helicity distributions in a broad kinematic range,
- novel electroweak structure functions,
- and the strangeness and anti-strangeness polarizations.

The latest status of global QCD fits to helicity dependent parton densities, which is not expected to improve much by the time the EIC would turn on, and the set of questions we want to address at the EIC are laid out in some detail in Sec. 1.10,

Precise measurements of the polarized structure function $g_{1}$ in a wide kinematic range will be a flagship measurement for the EIC. The gluon helicity distribution $\Delta g$ is strongly correlated with QCD scaling violations, i.e., the $Q$ dependence of $g_{1}$ at a given $x$. This will allow for a determination of $\Delta g$ down to unprecedented small values of $x$ of about $10^{-4}$. This in turn will eventually pinpoint the elusive gluon contribution to the spin of the proton, given by the integral of $\Delta g$ over all momentum fractions $x$, to about $10 \%$ accuracy or better. The striking quantitative impact on extractions of $\Delta g$ based on projected EIC data is demonstrated in Sec. 1.11. The same set of inclusive measurements will also provide a significantly better determination of the total quark contribution $\Delta \Sigma$ both as function of $x$ and the integral relevant for the nucleon spin sum.

Like in the unpolarized case, see Sec. 1.5, the best strategy to achieve a full flavor and quark-antiquark separation of polarized helicity densities is based again on semi-inclusive deep-inelastic hadron production. The kinematic coverage in $x$ and $Q$ is similar to what can be achieved in inclusive DIS, with the extra theoretical complication of the need for fragmentation functions to model hadronization. At medium-to-large values of $x$ one can address with precision certain interesting asymmetries in the polarized quark sea like $\Delta \bar{u}$ $\Delta \bar{d}$ (from charged pion yields) and perhaps even $\Delta s-\Delta \bar{s}$ (from charged kaon yields). The first quantity is predicted to be sizable in several model calculations of the nucleon but the precision of current experiments only gives a first hint of a possible non-zero asymmetry; the latter quantity may help to understand why the sum $\Delta s+\Delta \bar{s}$ appears to be much smaller in current experiments than expected. If $\Delta s$ and $\Delta \bar{s}$ have their spins anti-aligned, their sum could be small but the asymmetry would be sizable. Constraints from hyperon decay matrix elements and arguments based on $\mathrm{SU}(3)$ symmetry predict a significantly negative total ( $x$ integrated) strange quark polarization. To address the validity of this constraint and to access to what extent $\operatorname{SU}(3)$ symmetry is broken, one needs to determine $\Delta s$ down to small values of $x$ to obtain a reliable estimate of its $x$ integral. This is another unique measurement to be performed at the EIC.

First simulations of electroweak neutral and charged current deep-inelastic scattering at the EIC in Sec. 1.12 show that such measurements become feasible already with relatively modest integrated luminosities. The corresponding structure functions for polarized protons have never been measured before and probe combinations of quark flavors other than in one-photon-exchange dominating at low $Q$. To fully exploit the potential of the EIC for such measurements, positron beams are required, albeit not necessarily polarized. An effective source of polarized neutrons such as a Helium-3 beam would be highly desirable. When combined, these measurements will greatly aid the flavor decomposition of polarized parton densities at medium-to-large $x$, free of any hadronization ambiguities. At the highest c.m.s. energies and luminosities also photon- $Z$ boson interference contributions to structure functions should be accessible at the EIC. The production of charmed mesons in charged current DIS events is an alternative probe for the strange and anti-strange densities both unpolarized and polarized. This is discussed in Sec. 1.13

Table 1.1 summarizes the identified golden measurements, science deliverables, and experimental requirements in spin-dependent lepton-proton collisions at an EIC. Other, second tier measurements with polarization involve the currently unknown charm contribution to the deep-inelastic structure function $g_{1}$ which offers sensitivity to $\Delta g$ through photon-gluon fusion. Some expectations can be found in Sec. 1.11. If an effective neutron beam is available one can also attempt to determine the fundamental Bjorken sum rule at a few percent level. The Bjorken sum is probably one of the most precisely calculated quantities in perturbative QCD and provides an interesting link to the Adler $D$ function in electron-positron

| Deliverables | Observables | What we learn | Requirements |
| :---: | :---: | :---: | :---: |
| polarized gluon | scaling violations | gluon contribution | coverage down to $x \simeq 10^{-4} ;$ |
| distribution $\Delta g$ | in inclusive DIS | to proton spin | $\mathcal{L}$ of about $10 \mathrm{fb}^{-1}$ |
| polarized quark and <br> antiquark densities | semi-incl. DIS for <br> pions and kaons | quark contr. to proton spin; <br> asym. like $\Delta \bar{u}-\Delta \bar{d} ; \Delta s$ | similar to DIS; <br> good particle ID |
| novel electroweak <br> spin structure functions | inclusive DIS <br> at high $Q^{2}$ | flavor separation <br> at medium $x$ and large $Q^{2}$ | $\sqrt{s} \gtrsim 100 \mathrm{GeV} ; \mathcal{L} \gtrsim 10 \mathrm{fb}^{-1}$ <br> positrons; polarized ${ }^{3} \mathrm{He}$ beam |

Table 1.1. Golden measurements in polarized ep collisions at an EIC.
annihilation through the Crewther relation.
Finally, the production of hadronic final states in electron-proton collisions is dominated by the exchange of photons of almost zero virtuality. Photoproduction measurements and, in particular, the exploration of kinematic regimes where "resolved photon" contributions dominate was one of the great successes of the HERA physics program. Resolved processes, where the photon interacts with the proton through its non-perturbative source of partons, offer a fresh look at these densities which are so far mainly determined from imprecise LEP data. Given the anticipated high luminosity, an EIC can elevate these studies to a level of unprecedented precision, and, thanks to the polarized beams, allows one to investigate for the first time also the non-perturbative structure of circularly polarized photons. A good knowledge of the partonic structure of photons is essential for part of the physics program of a possible future linear collider. The general framework for photoproduction and two examples of physics studies are presented in Secs. 1.14 .1 .16 ,

To summarize, the physics goals of the EIC should be ambitious and must offer detailed answers to all the open fundamental questions concerning the spin and flavor structure of nucleons laid out above. The following sections will outline the path to achieve these goals. The program bears significant experimental challenges which all need to be carefully addressed to reach the desired unprecedented level of precision. With the exception of some of the electroweak structure function measurements, most observables will be quickly limited by systematic uncertainties, intrinsic ambiguities of the extraction method like, for instance, the Rosenbluth separation for $F_{L}$, and the way how well we can control QED radiative corrections to unfold the information one is actually interested in. Experimental aspects are discussed in Chapter 7.

### 1.2 Status of perturbative QCD calculations

Sven-Olaf Koch

### 1.2.1 Introduction

Deep-inelastic scattering (DIS) and the observed scaling violations are at the very center of the formulation of QCD as the gauge theory of the strong interactions [1, 2].

Over the decades the experiments using lepton and neutrino scattering off fixed targets at CERN, FNAL, SLAC, and JLAB as well as electron-proton collisions at the HERA collider at DESY have provided unique insight into the nucleon structure with the available high precision experimental data spanning a large kinematical range. Dramatic further improvements can be expected from the planned electron-ion collider EIC.

The key observables are either inclusive structure functions or differential cross sections in the semi-inclusive case, which parametrize the hard hadronic interaction in the QCD improved parton model. The particle data group (PDG) 3 provides a very readable account of DIS, including the definitions of kinematic variables, etc.


Figure 1.1. QCD factorization of the cross section for the scattering of a deeply virtual boson with (space-like) momentum $q\left(-q^{2}=Q^{2}>0\right)$ off a proton with momentum $P$ in their center-of-mass frame, see Eq. (1.1).

Precision predictions in perturbative QCD rest on the fact that we can separate the sensitivity to dynamics from different scales, i.e., the physics at scale of the proton mass from hard, high-energy scattering at a large scale $Q^{2}$. For lepton-proton DIS in the one-boson exchange approximation this is depicted in Fig. 1.1. For unpolarized DIS, this factorization at a scale $\mu$ allows to express the structure functions $F_{k}(k=2,3, L)$ as convolutions of parton distributions (PDFs) $f_{i}(i=q, \bar{q}, g)$ and short-distance Wilson coefficient functions $C_{k, i}$,

$$
\begin{equation*}
F_{k}\left(x, Q^{2}\right)=\sum_{i=q, \bar{q}, g} \int_{x}^{1} d z f_{i}\left(\frac{x}{z}, \mu^{2}\right) C_{k, i}\left(z, Q^{2}, \alpha_{s}(\mu), \mu^{2}\right), \tag{1.1}
\end{equation*}
$$

up to corrections of higher twist $\mathcal{O}\left(1 / Q^{2}\right)$. The coefficient functions $C_{k, i}$ are calculable perturbatively in QCD in powers of the strong coupling constant $\alpha_{s}$,

$$
\begin{equation*}
C=C^{(0)}+\alpha_{s} C^{(1)}+\alpha_{s}^{2} C^{(2)}+\alpha_{s}^{3} C^{(3)}+\ldots, \tag{1.2}
\end{equation*}
$$

with the expansion coefficients $C^{(0)}$ denoted as the leading order (LO), $C^{(1)}$ the next-toleading order (NLO) and so on. The PDFs $f_{i}$ describe the fraction $x=Q^{2} /(2 P \cdot q)$ of the nucleon momentum carried by the quark or gluon. PDFs are non-perturbative objects and have to be obtained from global fits to experimental data or determined, e.g., by lattice computations. Perturbation theory, however, provides information about their scale dependence, i.e., the well-known evolution equations,

$$
\frac{d}{d \ln \mu^{2}}\binom{f_{q_{i}}\left(x, \mu^{2}\right)}{f_{g}\left(x, \mu^{2}\right)}=\sum_{j} \int_{x}^{1} \frac{d z}{z}\left(\begin{array}{cc}
P_{q_{i} q_{j}}(z) & P_{q_{i} g}(z)  \tag{1.3}\\
P_{g q_{j}}(z) & P_{g g}(z)
\end{array}\right)\binom{f_{q_{j}}\left(x / z, \mu^{2}\right)}{f_{g}\left(x / z, \mu^{2}\right)}
$$

The splitting functions $P_{i j}$ are universal quantities in QCD and describe the different possible parton splittings in the collinear limit. Like the $C_{k, i}$ also the $P_{i j}$ can be computed in a power series in $\alpha_{s}$,

$$
\begin{equation*}
P=\alpha_{s} P^{(0)}+\alpha_{s}^{2} P^{(1)}+\alpha_{s}^{3} P^{(2)}+\ldots . \tag{1.4}
\end{equation*}
$$

Analogous formulae hold for the polarized DIS structure functions. In particular, for $g_{1}$ one may apply the obvious replacements $f_{i} \rightarrow \Delta f_{i}, C_{k, i} \rightarrow \Delta C_{g_{1}, i}$, and $P_{i j} \rightarrow \Delta P_{i j}$ in Eqs. (1.1)-(1.4). QCD factorization has also been established for (semi-)inclusive deepinelastic scattering (SIDIS), where the cross section $d^{2} \sigma / d x d Q^{2}$ is subject to a decomposition similar to Eq. (1.1). Although, in that case, the process dependent hard parton scattering cross sections need to be augmented by an additional prescription for the final state parton, e.g., a jet algorithm or fragmentation functions.

### 1.2.2 Current status

QCD predictions for DIS observables have reached over the years an unprecedented level of precision. All quantities in Eqs. (1.1)-(1.4) have been computed to higher orders in perturbation theory so that the effect of radiative corrections on those observables is well understood and largely under control. In the case of unpolarized DIS, the splitting functions $P_{i j}$ are known to NNLO [4, 5] and, likewise, the coefficient functions $C_{k, i}$ [6, 7, 8, 8]. For photon and charged current $W^{ \pm}$-boson exchange, even the hard corrections at order $\mathcal{O}\left(\alpha_{s}^{3}\right)$ are available [10, 11]. In the case of polarized DIS, the spin dependent splitting functions $\Delta P_{i j}$ at two loop order have been obtained some time ago [12, 13]. At NNLO, the polarized splitting functions $\Delta P_{q q}$ and $\Delta P_{q g}$ have been reported [14], and the coefficient functions $\Delta C_{g_{1}, i}$ are available from [15]. For semi-inclusive observables, the QCD corrections are typically known to NLO. This corresponds to $\mathcal{O}\left(\alpha_{s}^{2}\right)$ since the underlying Born cross section behaves as $d^{2} \sigma^{(0)} / d x d Q^{2} \sim \mathcal{O}\left(\alpha_{s}\right)$ due to the additional final state parton. Processes considered include, for instance, the electro-production of hadrons with high transverse momentum [16, 17] or single inclusive DIS jet cross sections [18].

The currently available QCD predictions for inclusive DIS and SIDIS put us in comfortable position to confront experimental data with theory at a very high level of precision. In these comparisons, we no longer test QCD. Rather we use perturbative QCD as an essential and established part of our theory toolkit to deduce important information about PDFs or the value of the strong coupling constant $\alpha_{s}\left(M_{Z}\right)$. Of course, this is a situation that, generally, needs to be addressed also beyond DIS, since experimental data from the unpolarized (anti-)proton-proton colliders Tevatron at FNAL and the LHC at CERN as well as from the polarized proton-proton collider RHIC at BNL help to further constrain the non-perturbative input to QCD precision predictions. See, e.g., the analyses of
unpolarized PDFs to NNLO in Refs. [19, 20, 21, 22] or recent studies of polarized PDFs in [23, 24, 25, 26, 27, 28].

Given the current status of perturbative QCD, experimental data from a future program of electron-ion collisions, EIC, can help to address and clarify a number of still open and yet very relevant questions; see also Secs. 1.4 and 1.11 . For the case of unpolarized PDFs improvements can be made with respect to the flavor asymmetry of sea quarks at low $x$ and the valence quarks at large $x$, by studying, e.g., electron-deuteron collisions. Much of the physics case here had already been investigated in an assessment of the experimental prospects of electron-deuteron scattering at HERA some time ago [29. More generally, the high luminosity of an EIC would further constrain PDFs, especially the gluon at low $x$ and $Q^{2}$. In this context, a precision measurements of the longitudinal structure function $F_{L}$, which is an observable predominantly driven by the gluon PDF is of high interest as it would complement and, eventually even supersede, existing experimental data, see, e.g., 30. New high statistics DIS experiments can also improve the current precision of strong coupling constant $\alpha_{s}$ measurements in space-like kinematics.

For polarized DIS, a very fundamental question still remains the understanding of the proton spin, in particular, whether the polarized gluon PDF $\Delta f_{g}$ provides a significant contribution. To that end, an extension of the kinematical coverage in $x$ and $Q^{2}$, as it could be achieved by an electron-ion collider, is of paramount importance. This would help to access higher scales in $Q^{2}$ in order to test the perturbative evolution Eq. (1.3). Likewise, access to an extended $x$-range allows for a better determination of moments of the $\Delta f_{i}$. They also enter, e.g., in the Bjorken sum rule for polarized electro-production, which is again an observable very well-known in perturbative QCD [31, 32]. Other issues of interest for polarized DIS in electron-ion collisions concern a reliable extraction of flavor structure as well as a study of strangeness PDFs, $\Delta f_{s}$.

### 1.2.3 Summary

We have briefly summarized the current status of perturbative QCD predictions for DIS experiments. To date, we can build on a very mature understanding of the theory, which could be confronted with experimental data from a future electron-ion collider in order to improve our knowledge about the fundamental structure of matter and the important dynamics of quarks and gluons in nucleons.

### 1.3 Unpolarized proton structure - HERA's legacy

Amanda Cooper-Sarkar (for the H1 and ZEUS Collaborations)

### 1.3.1 Introduction

HERA data provide the most insight into the behaviour of unpolarized parton distribution functions (PDFs) at present and as such represent an integral part of all global QCD analyses. The H1 and ZEUS experiments are combining their various sub-sets of data so as to provide a legacy of HERA results. The combination of inclusive cross section data from HERA-I and the PDF fit based on these data are already published [20]. In 2010 further data have been combined and PDF fits to the augmented data sets have been made available in preliminary form. In Sec. 1.3 .2 results from the published combination are reviewed. In Sec. 1.3.3 results from a combination of $F_{2}^{c \bar{c}}$ data are presented and their sensitivity to the mass of the charm quark and the choice of the heavy flavor scheme adopted in the global PDF fit is discussed. In Sec. 1.3.4 results from the combination of inclusive cross section data taken at lower proton beam energies are discussed. Finally, in Sec. 1.3 .5 an updated combination of all inclusive data from HERA-I and HERA-II running is shown and a PDF fit to these data is presented.

### 1.3.2 Inclusive data from HERA-I running (1992-2001)

The inclusive cross section data, from the HERA-I running period, for Neutral Current ( $\mathrm{NC)} \mathrm{and} \mathrm{Charged} \mathrm{Current} \mathrm{(NC)}, e^{+} p$ and $e^{-} p$ scattering have been combined 20]. The combination procedure pays particular attention to the correlated systematic uncertainties of the data sets such that resulting combined data benefits from the best features of each detector. The combined data set has systematic uncertainties which are smaller than its statistical errors and the total uncertainties are small ( $1-2 \%$ ) over a large part of the kinematic plane. The combined data is compared to the separate input data sets of ZEUS and H1 in Fig. 1.2 ,

These data are used as the sole input to a PDF fit called the HERAPDF1.0 [20. The motivations for performing a HERA-only fit are firstly, that the combination of the HERA data yields a very accurate and consistent data set such that the experimental uncertainties on the PDFs may be estimated from the conventional $\chi^{2}$ criterion $\Delta \chi^{2}=1$. Global fits which include dats sets from many different experiments often use inflated $\chi^{2}$ tolerances in order to account for marginal consistency of the input data sets. Secondly, the HERA data are proton target data so that there is no uncertainty from heavy target corrections or deuterium corrections and there is no need to assume that $d$ in the proton is the same as $u$ in the neutron since the $d$-quark PDF may be extracted from $e^{+} p$ CC data. Thirdly, the HERA inclusive data give information on the gluon, the Sea and the $u$ - and $d$-valence PDFs over a wide kinematic region: the low- $Q^{2} \mathrm{NC} e^{+} p$ cross-section data are closely related to the low- $x$ Sea PDF and the low- $x$ gluon PDF is derived from its scaling violations; the high$x u-$ and $d$-valence PDFs are closely related to the high- $Q^{2} \mathrm{NC} e^{ \pm} p, \mathrm{CC} e^{-} p$, and $\mathrm{CC} e^{+} p$ cross sections, respectively; the difference between the high- $Q^{2} e^{-} p$ and $e^{+} p$ cross-sections gives the valence shapes down to low $x, x \sim 10^{-2}$.

HERAPDF provides model and parametrisation uncertainties on the PDFs as well as experimental uncertainties; for details, see Ref. [20]. A major contribution to the total uncertainties in the HERAPDF1.0 set comes from the model uncertainty on the charm mass value. This can be improved using information from data on $F_{2}^{c \bar{c}}$.


Figure 1.2. HERA combined data points for the NC $e^{+} p$ cross section as a function of $Q^{2}$ in selected bins of $x$, compared to the separate ZEUS and H1 data sets input to the combination.

### 1.3.3 Charm data from HERA-I and II running

H1 and ZEUS have also combined their data on $F_{2}^{c \bar{c}}$ [20]. In Fig. 1.3 the combined data are compared to the separate data sets which go into the combination. These data are input to the HERAPDF fit together with the inclusive data which were used for HERAPDF1.0. The $\chi^{2}$ of this fit is sensitive to the value of the charm quark mass. Fig. 1.4 compares the $\chi^{2}$, as a function of this mass, for a fit which includes these data (left) to that for the HERAPDF1.0 fit (middle). However, it would be premature to conclude that the data can be used to determine the charm pole-mass. The HERAPDF formalism uses the ThorneRoberts (RT) variable-flavour-number (VFN) scheme for heavy quarks. This scheme is not unique, specific choices are made for threshold behaviour. In Fig. 1.4 (right) the $\chi^{2}$ profiles for the standard and the optimized versions of this scheme are compared to two alternative ACOT VFN schemes and the Zero-Mass VFN scheme. Each of these schemes favours a different value for the charm quark mass, and the fit to the data is equally good for all the heavy quark mass schemes; see Fig. 1.3 (right). However, the Zero-Mass scheme is $\chi^{2}$ disfavoured; see Ref. [20] for further details.

### 1.3.4 Low energy proton beam data from 2007

In $2007 \mathrm{NC} e^{+} p$ data were taken at two lower values of the proton beam energy in order to determine the longitudinal strucure function $F_{L}$. Some of the H1 and ZEUS data sets from these runs have now been combined [20] and the results for the $\mathrm{NC} e^{+} p$ cross section are shown in Fig. 1.5. These data have been input to the HERAPDF fit together with the inclusive data from HERA-I. The resulting PDFs are compared with those of HERAPDF1.0 in Fig. 1.5, The low energy data are sensitive to the choice of minimum $Q^{2}$ (standard cut $Q^{2}>3.5 \mathrm{GeV}^{2}$ ) for data entering the fit. If a somewhat harder cut, $Q^{2}>5 \mathrm{GeV}^{2}$, is made, a steeper gluon distribution results, see Fig. 1.5, whereas for the HERAPDF1.0 this variation of cuts results in PDFs which lie within the PDF uncertainty bands. This sensitivity is also present if an $x$ cut, $x>5 \times 10^{-4}$, or a "saturation inspired" cut, $Q^{2}>0.5 x^{-0.3}$, is made. This sensitivity may indicate the breakdown of the DGLAP formalism at low $x$ [33].


Figure 1.3. Left: HERA combined data points for $F_{2}^{c \bar{c}}$ compared to the separate ZEUS and H1 data sets. Right: HERA combined data points for $F_{2}^{c \bar{c}}$ compared to HERAPDF fits to these plus the inclusive DIS data, for various different heavy-quark-mass schemes.


Figure 1.4. The $\chi^{2}$ of the HERAPDF fit as a function of the charm mass $m_{c}^{\text {model }}$. Left and Middle: using the RT-standard scheme, when $F_{2}^{c \bar{c}}$ data are not included and included in the fit, respectively. Right: results for using various mass schemes in the fit to $F_{2}^{c \bar{c}}$ data.


Figure 1.5. Left: HERA combined data points for the $\mathrm{NC} e^{+} p$ cross-section for three different proton beam energies. Right: PDFs, $x u_{v}, x d_{v}, x S=2 x(\bar{U}+\bar{D})$, and $x g$ at $Q^{2}=10 \mathrm{GeV}^{2}$, for HERAPDF1.0 and for a HERAPDF fit which also includes the low-energy proton beam data, with the standard $Q^{2}$ cut, $Q^{2}>3.5 \mathrm{GeV}^{2}$, and for $Q^{2}>5.0 \mathrm{GeV}^{2}$.

### 1.3.5 High- $Q^{2}$ data from HERA-II running

Preliminary H1 data on NC and $\mathrm{CC} e^{+} p$ and $e^{-} p$ inclusive cross-sections and published ZEUS data on NC and CC $e^{-} p$ and CC $e^{+} p$ data, from HERA-II running, have been combined with the HERA-I data to yield an inclusive data set with improved accuracy at high $Q^{2}$ and high $x[34]$. The HERA-I data set and the new HERA I+II data sets are compared for CC $e^{-} p$ data in Fig. 1.6. This new data set is used as the sole input to a new PDF fit called the HERAPDF1.5 which uses the same formalism and assumptions as the HERAPDF1.0 fit [35]. These fits are superimposed on the corresponding data sets in the figure. Fig. 1.7 (left) shows the combined data for $\mathrm{NC} e^{ \pm} p$ cross-sections with the HERAPDF1.5 fit superimposed. The PDFs from HERAPDF1.0 and HERAPDF1.5 are compared in Fig. 1.7 (right). The improvement in precision at high $x$ is clearly visible.

### 1.3.6 Summary

The status of the combinations of H1 and ZEUS data has been discussed. HERA leaves rich legacy of results which are the basis for all present QCD analyses of unpolarized PDFs and define the goals for any future DIS experiment.


Figure 1.6. HERA combined data points for the CC $e^{-} p$ cross-section. Left: from the HERA-I run period. Right: from the HERA-I and II run periods. On each plot the HERAPDF fit which includes the corresponding data is illustrated: the HERAPDF1.0 fit on the left hand plot and the HERAPDF1.5 on the right hand plot.


Figure 1.7. Left: HERA combined data points for the NC $e^{ \pm} p$ cross-sections for data from the HERA-I and II run periods. The HERAPDF1.5 fit to these data is also shown on the plot. Right: Parton distribution functions from HERAPDF1.0 and HERAPDF1.5; $x u_{v}, x d_{v}, x S=2 x(\bar{U}+\bar{D})$ and $x g$ at $Q^{2}=10 \mathrm{GeV}^{2}$.

# 1.4 Unpolarized parton distribution functions: questions to be addressed at an EIC 

Marco Guzzi, Pavel Nadolsky, Fredrick Olness

### 1.4.1 Introduction

The Electron-Ion Collider (EIC) will operate at a time when the Large Hadron Collider (LHC) has established a new "gold standard" for perturbative QCD by measuring a variety of hard-scattering processes. High-luminosity EIC measurements will be very complementary to those at the LHC, as they will accurately probe various aspects of hadronic structure using independent experimental techniques. In the next few years, when next-to-next-to-leading order (NNLO) accuracy of QCD calculations becomes the norm, a variety of perturbative and nonperturbative effects need to be taken into account to match the precision of multi-loop radiative contributions. Some of these effects can be constrained solely by the LHC data; others need independent measurements, not affected by systematical uncertainties present at the LHC. With an integrated luminosity of $10 \mathrm{fb}^{-1}$ or more, the EIC will disentangle many such effects, including modifications of the nucleon structure within heavy-nuclei targets, flavor dependence of parton distribution functions (PDFs), and QCD dynamics at very large or small $x$.

As compared with previous lepton-nucleus experiments, the EIC will probe to smaller $x$ values with high precision. In contrast to the HERA ep collider, which explores the same $\left\{x, Q^{2}\right\}$ region, heavy-ion scattering will achieve much higher partonic densities that are a prerequisite for the onset of saturation. It will help delineate the kinematical boundary between the DGLAP factorization and saturated dynamics in the nuclear medium.

The $Q^{2}$ range of the EIC will cover the transition region from the perturbative to the non-perturbative regime. Here, we wish to learn how the perturbative parton-scattering picture valid at large momentum transfers matches on nonperturbative models describing the strongly-coupled resonance region. Understanding of this region is important for hadronic experiments at the intensity frontier.

### 1.4.2 Open Questions

Several questions about PDFs will likely remain open at the time of the EIC operation. Figure 1.8 shows the kinematic domains in $x$ and $Q^{2}$ probed by current experiment and the PDFs that are most strongly constrained in these reqions.

Nuclear PDFs. Several groups extract nuclear PDFs and their uncertainties by analyzing the global data on nuclear targets [36, 37, 38, 39, 40]. In their studies, they find that the nuclear corrections depend on the type of the nucleus (its atomic number $A$ ), flavor of the probed parton, and even the type of the probing boson. For example, it was found recently [41, 37] that the nuclear correction factors preferred by the $\nu \mathrm{Fe}$ DIS data by NuTeV [42] are surprisingly different from predictions based on the $\ell^{ \pm} \mathrm{Fe}$ charged-lepton results.

By performing deep inelastic scattering (DIS) both on proton and heavy-nuclei targets, the EIC can distinguish between intrinsic properties of the proton and those of the extended nuclear medium. A high-intensity EIC could use a variety of nuclear beams to precisely map the $A$-dependent nuclear correction factors in the $\left\{x, Q^{2}\right\}$ kinematic plane and clarify the behavior of nuclear corrections to NC DIS. Such information is of importance for determining the proton PDFs, in particular, the strange quark PDF that is constrained largely


Figure 1.8. Kinematic domains in $x$ and $Q^{2}$ probed by fixed-target and collider experiments, shown together with the PDFs that are most strongly constrained by the indicated regions [3]. DIS data off nuclear targets exist only in the fixed-target region.
from the NuTeV data. The nuclear correction affects the uncertainty in $s(x, Q)$, which is large at present and may limit the precision of electroweak studies in $W$ and $Z$ boson production at the LHC [43].

The topics of nuclear PDFs and saturation will be extensively discussed in the Chapter 5 devoted to $e A$ physics at an EIC.

Better constraints on the strangeness PDF. Despite extensive investigation, there remain large uncertainties in flavor differentiation of sea-quark PDFs both in the proton and nuclei. In particular, the strange quark+antiquark distribution in the proton, $s_{+}(x)=$ $s(x)+\bar{s}(x)$, and its asymmetry, $s_{-}(x)=s(x)-\bar{s}(x)$, are still poorly known [44, 45, 46, 22, 47, despite their significance for understanding of the nucleon structure. Existing constraints on the strangeness come predominantly from neutrino (semi-)inclusive DIS [48, 42]. At the EIC, both $s_{+}(x)$ and $s_{-}(x)$ can be probed in semi-inclusive DIS production of kaons; see Sec. 1.5 for some quantitative studies. This measurement will rely on a good understanding of fragmentation functions, which will be known much better by the time an EIC turns on.

The $d / u$ ratio at large $\mathbf{x}$. Because of its intermediate energy and high beam intensity, the EIC is ideal for studying parton distributions at large Bjorken $x(x>0.1)$, where separation of parton flavors is not fully understood despite many years of experiments. For example, even the ratio $d(x, Q) / u(x, Q)$ of the dominant up and down quark proton PDFs at $x>0.3$ has been recently put in doubt by contradicting constraints from DIS on deuteron targets [49, 50] and charged lepton asymmetry at the Tevatron [51, 52]. While the PDF analysis groups labor to understand these differences [22, 46, 53 (and new clean LHC measurements of the $d / u$ ratio in proton scattering are in the queue), the EIC will help to resolve this controversy by extracting the ratio $F_{2}^{n}(x, Q) / F_{2}^{p}(x, Q)$ from DIS data on various nuclear targets. Such measurement will help to separate several types of kinematical and nuclear corrections ([54], and references therein) that influence the $F_{2}^{n} / F_{2}^{p}$ ratio derived
from nuclear-target DIS.
Gluon PDF in the proton and charm production at large x. Even more uncertainty exists in the gluon $\operatorname{PDF} g(x, Q)$ at large $x$, where it can be larger than the down-quark $d(x, Q)$ at $x>0.5$ in some recent parametrizations for proton PDFs [55]. This ambiguity will be reduced by upcoming high- $p_{T}$ jet production at the LHC, but significant systematic limitations of both experimental and theoretical nature may persistent at the largest $x$, where the EIC could independently contribute. Production of heavy-quark $(c, b)$ pairs or heavy mesons $(J / \psi, \Upsilon)$ in deep-inelastic scattering could accurately probe the large- $x$ gluon PDF. The EIC detectors will have excellent charm tagging efficiency, in a relatively clean scattering environment as compared to the LHC.

Inclusive charm production is interesting in its own right, given that large radiative contributions are known to exist near the heavy-quark production threshold, i.e., at $Q$ comparable to the charm quark mass; see Sec. 1.7 for a detailed account of heavy quark contributions to DIS structure functions. The rate for charm production at large $x, x \gtrsim 0.1$, can be increased by up to an order of magnitude by nonperturbative intrinsic charm production suggested by light-cone models [56, 57]. An EIC will be a unique opportunity to cleanly test for the presence of intrinsic charm contributions; see Sec. 1.9 for some quantitative studies.

Transition to the high-density regime. There is a long-standing question of partonic saturation and recombination in the small- $x$ region. As a related phenomenon, BFKL [58, [59, 60] effects from large $\ln [1 / x]$ contributions may supersede the usual DGLAP evolution in the small-x regime. The EIC should be capable of probing the transition from DGLAP factorization to BFKL/saturation dynamics, particularly using heavy nuclei beams in order to produce large partonic densities; see Chapter 5 for details on $e A$ physics.

Perturbative-nonperturbative QCD boundary. The general kinematic parameters of an EIC would span across both the perturbative (large $Q^{2}$ ) region and the nonperturbative (small $Q^{2}$ ) region. The theoretical description of the physics in these two regions is very different, and precise EIC data might enable us to better connect these two disparate theoretical descriptions.

The longitudinal structure function. The longitudinal structure function $F_{L}=$ $F_{2}-2 x F_{1}$ is of special interest, in view that its leading $\mathcal{O}(1)$ term vanishes according to the Callan-Gross relation. The first non-vanishing, leading order contribution is of $\mathcal{O}\left(\alpha_{s}\right)$ and dominated by photon-gluon fusion. Hence, $F_{L}$ is particularly sensitive to the gluon distribution $g\left(x, Q^{2}\right)$. Corrections up to $\mathcal{O}\left(\alpha_{s}^{3}\right)$ are known [10, allowing for a consistent analysis of $F_{L}$ at NNLO accuracy. An EIC could make the first precise measurements of $F_{L}$ in a kinematic range that overlaps both the fixed-target and HERA collider data 30 which have large statistical uncertainties; see Sec. 1.6 for more details on such a measurement at an EIC.

Electroweak contributions to proton PDFs. Some, if not all, NLO electroweak effects will be included in future PDF analyses, as their magnitude is comparable to the size of NNLO QCD radiative contributions that will be routinely included. The QCD+EW PDFs require additional experimental input to constrain nonperturbative parametrizations for photon PDFs, as well as charge asymmetry effects (isospin violation) between PDFs for up-type quarks and down-type quarks at the initial scale $Q \approx 1 \mathrm{GeV}$. An EIC has the potential to contribute toward improving limits on electroweak PDF terms either directly or in combination with neutrino DIS measurements.

When extracting information about the proton PDFs from scattering on nuclear targets, we generally make use of isospin symmetry to relate the proton and neutron PDFs via a
$u \leftrightarrow d$ interchange. While the isospin symmetry is elegant, it is nonetheless approximate and can be violated at the level of a few percent [61, 62, 63, 64, 65, 66, 67, 41, 68]. Violation of the exact $p \leftrightarrow n$ isospin symmetry, or charge symmetry violation (CSV), invalidates the parton model relations that reduce the number of independent nonperturbative distributions; e.g., $u^{n}(x) \not \equiv d^{p}(x)$ and $u^{p}(x) \not \equiv d^{n}(x)$. It is important to be aware of the potential magnitude of isospin symmetry violation and its consequences for flavor separation of proton PDFs.

It is noteworthy that isospin symmetry is automatically violated both perturbatively and nonperturbatively. This is because the photon couples to the up quark distribution $u^{p}(x)$ differently than to the down quark distribution $d^{n}(x)$. These terms can be comparable to the NNLO DGLAP evolution effects [69, 70, 71].

Some combinations of structure functions, such as $\Delta F_{2} \equiv \frac{5}{18} F_{2}^{C C}\left(x, Q^{2}\right)-F_{2}^{N C}\left(x, Q^{2}\right)$ and $\Delta x F_{3}=x F_{3}^{W^{+}}-x F_{3}^{W^{-}}$, can be particularly sensitive to isospin violations, and an EIC can contribute to their measurement. For example, the EIC is capable of measuring precisely the structure function $F_{2}^{N C}$ mediated by the neutral-current $\gamma / Z$ exchange processes. Measurement of $F_{2}^{C C}$, mediated by the charged-current $W^{ \pm}$exchange, would rely on compensating the $M_{W}^{2} / Q^{2}$ suppression of the $W$ boson propagator with high intensity of the beams; see Sec. 1.12 for more details on electroweak structure function measurements at an EIC.

In separate experiments, $\Delta x F_{3}$ can be measured precisely via the neutrino-nucleon DIS process; as these measurements are performed with heavy nuclear targets, the nuclear correction factors can be the limiting factor as to the derived CSV constraint. Since an EIC will use a variety of nuclear targets, it can obtain very precise nuclear correction factors; this information could, in principle, be used together with the neutrino-nucleon DIS data to extract improved CSV limits.

The structure functions $\Delta F_{2}$ and $\Delta x F_{3}$ receive contributions from both heavy flavors as well as CSV contributions; improved understanding of the heavy-quark components (discussed previously) can indirectly contribute to better CSV limits 68].

The combination of high-statistics EIC measurements and constraints could thus yield important information on the fundamental charge symmetry.

### 1.4.3 Acknowledgments

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### 1.5 Flavor separation from semi-inclusive DIS

Elke-Caroline Aschenauer, Marco Stratmann

### 1.5.1 Motivation and Method

The strangeness distribution and a possible asymmetry between strangeness and antistrangeness densities have been identified as two of the most compelling open questions in hadronic physics which are difficult to address without an EIC; see Sec. 1.4.

Existing constraints in global fits come predominantly from neutrino (semi-)inclusive DIS 48, 42] but both $s_{+}(x) \equiv s(x)+\bar{s}(x)$ and $s_{-}(x) \equiv s(x)-\bar{s}(x)$ are still only poorly known [46, 22, 72]. Figure 1.9 summarizes recent uncertainty estimates for $s_{ \pm}$from three global QCD fits.


Figure 1.9. Uncertainty bands for $s_{ \pm}$at $Q^{2}=2 \mathrm{GeV}^{2}$ for recent fits. Figure taken from [72].
Semi-inclusive DIS with identified charged kaons is expected to be a viable method to determine the elusive strange quark density and perhaps a possible asymmetry $s_{-}$experimentally. One can access basically the same a broad kinematic range in $x$ and $Q^{2}$ as in inclusive DIS. The HERMES collaboration has successfully performed such a measurement in the range $0.02<x<0.6$ at an average $Q^{2}$ of about 2.5 GeV [73]. Compared to $s(x)$ from most global PDF fits, they find a softer strangeness distribution in their LO analysis. Clearly, more data in a larger range of $x$ and $Q^{2}$ are necessary to clarify this issue.

The SIDIS measurement relies, however, on a good understanding of the hadronization mechanism which is encoded in non-perturbative, collinear parton-to-hadron fragmentation functions (FFs) $D_{i}^{H}$ if factorization is assumed in a pQCD calculation. Like PDFs, FFs are extracted from global QCD analyses. One can resort to a wealth of single-inclusive hadron production data obtained at different c.m.s. energies in $e^{+} e^{-}$annihilation and in $e p$ and $p p(p \bar{p})$ scattering. Pion FFs are currently known best with uncertainties of about $5 \div 10 \%$ depending on the flavor of the fragmenting parton [74]. Ambiguities for kaon FFs are about twice as large [74]. Significant progress on the quality of fits to FFs is expected once data from $B$ factories and the LHC become available. Also, NNLO evolution kernels are expected to become available in the near future [75], which will help to reduce theoretical scale ambiguities further.

All relevant SIDIS cross sections are known at least to NLO accuracy [76, 77, 78, 79], and the analytical expressions are relatively simple and easy to implement into global fits of PDFs, see, e.g., [80]. Schematically the unpolarized SIDIS cross section for the production of a hadron $H$ in the current fragmentation region reads

$$
\begin{equation*}
\frac{d \sigma^{H}}{d x d y d z}=\frac{2 \pi \alpha^{2}}{Q^{2}}\left[\frac{1+(1-y)^{2}}{y} 2 F_{1}^{H}\left(x, z, Q^{2}\right)+\frac{2(1-y)}{y} F_{L}^{H}\left(x, z, Q^{2}\right)\right] \tag{1.5}
\end{equation*}
$$

with $x$ and $y$ denoting the usual DIS variables, $-q^{2}=Q^{2}=S x y$, and $z=p_{H} \cdot p / p \cdot q$ the momentum fraction taken by the hadron $H$. Assuming factorization, the structure functions $F_{1, L}^{H}$ at a factorization scale $\mu \sim Q$ can be expressed as convolutions of non-perturbative PDFs $f_{j}(x, \mu)$ and FFs $D_{i}^{H}(z, \mu)$ with short-distance Wilson coefficients $C_{i j}^{1, L}(x, z, \mu)$.

### 1.5.2 Expectations for Charged Kaon Production at an EIC

Figures 1.10 and 1.11 show expectations for the $K^{+}$and $K^{-}$production cross section (1.5) at NLO accuracy, respectively, as a function of $x$ in bins of $Q^{2}$, using $0.01 \leq y \leq 0.95$ and $\sqrt{S}=70.7 \mathrm{GeV}$ (i.e., $5 \times 250 \mathrm{GeV}$ collisions at an EIC). To reduce uncertainties from kaon FFs, $z$ is integrated in the range $0.2 \leq z \leq 0.8$. The DSS set 74 is used. The solid lines are the statistical average over 100 replicas in the NNPDF2.0 neural network analysis [47] and the dashed lines reflect the corresponding PDF uncertainties.

Also shown in Figs. 1.10 and 1.11 are simulations based on the PYTHIA 81 event generator in the same kinematic range. Here, the CTEQ6L set of PDFs [82] has been used. The hadronic final state was simulated using JETSET based on LEP fragmentation settings and a suppression of $s \bar{s}$ pair production from the vacuum of 0.3 [PARJ (2)] compared to $u \bar{u}$ or $d \bar{d}$ creation. The results turn out to be remarkably similar to the NLO calculations based on collinear factorization despite the very different way hadronization is implemented in PYTHIA and the fact that only LO matrix elements are used, albeit matched with a parton shower. This gives us quite some confidence that the PYTHIA generator can be used to provide very reasonable estimates of yields for DIS-type processes at an EIC. In addition, it also tells us that the current DSS kaon FFs are doing a good job and include a realistic amount of "strangeness suppression". Already after one month of operation, corresponding to an integrated luminosity of about $20 \mathrm{fb}^{-1}$ the measurement will be limited by systematic uncertainties which need to be carefully studied. The statistical accuracy is significantly better than indicated by size of the points shown in the figures.

If one compares the results for $K^{+}$and $K^{-}$in Figs. 1.10 and 1.11 one finds hardly any difference at the smallest $x$ values in each $Q^{2}$ bin. At larger $x$ values, where $s_{-}$is largest, see Fig. [1.9, the yields for $K^{-}$are significantly lower than the ones for $K^{+}$. An EIC should be able to provide accurate measurements of both $s_{+}$and $s_{-}$in a broad kinematic range up to $Q^{2}$ values of a few hundred GeV .

Within the neural network approach it is in principle fairly straightforward to quantify by how much a new data set will reduce present PDF uncertainties. The original ensemble of replicas is constructed in such a way that all have the same weight. Information contained in new data sets can be incorporated without the need for refitting by reweighting each PDF in the ensemble by the probability that it agrees with the new data [47, 53]. Sets with small weights will become largely irrelevant in statistical averages. If too many sets receive small weights the accuracy of results from the new PDF ensemble will deteriorate, and the reweighting procedure becomes unreliable, necessitating a full refit. One reason for this to happen is, that the new data set contains significant new information which leads to much smaller uncertainties in certain kinematic regions. This is exactly what happens when one applies the reweighting method to the SIDIS data shown in Figs. 1.10 and 1.11 even if one assigns a fictitious $\mathcal{O}(5 \%)$ systematic uncertainty to each data point.

There are many other things which can be studied in SIDIS at an EIC. For instance, one can also bin in $z$ which makes the measurement more sensitive to the shape of the kaon FFs. This will provide a more stringent check whether FFs are universal functions in $e^{+} e^{-}, e p$, and $p p$ scattering. Pion yields will allow one to study other interesting and
relevant PDF combinations such as $\bar{u}(x)-\bar{d}(x)$. Similar measurements can be also done with longitudinally polarized beams which will give access to the helicity-dependent quark and antiquark densities, see Sec. 1.11. Detailed quantitative studies including more timeconsuming global QCD analyses with simulated SIDIS data for various c.m.s. energies are planned to quantify the impact of such measurements on our understanding of the spin and flavor structure of the nucleon. These studies should include also some estimates of the various sources of systematic uncertainties, like detector resolution, uncertainties in the particle identification, luminosity, and polarization measurements, details on these can be found in Sec. 7.3.


Figure 1.10. SIDIS cross section for $K^{+}$production at NLO accuracy using NNPDF2.0 PDFs 47. The dashed lines denote the PDF uncertainties. Also shown (points) are the results from a PYTHIA simulation (see text).


Figure 1.11. Same as in Fig. 1.10 but now for $K^{-}$production.

### 1.6 The longitudinal structure function $F_{L}$ at an EIC

Elke C. Aschenauer, Ramiro Debbe, Marco Stratmann

### 1.6.1 Motivation and Current Status of $F_{L}$ Results

The DIS reduced cross section $\sigma_{r}$ for one-photon-exchange can be represented as the sum of two independent structure functions $F_{2}$ and $F_{L}$ as follows

$$
\begin{equation*}
\sigma_{r} \equiv \frac{Q^{4} x}{2 \pi \alpha_{e m}^{2} Y_{+}} \frac{d^{2} \sigma}{d x d Q^{2}}=F_{2}\left(x, Q^{2}\right)-\frac{y^{2}}{Y_{+}} F_{L}\left(x, Q^{2}\right) \tag{1.6}
\end{equation*}
$$

where $Y_{+} \equiv 1+(1-y)^{2}$ depends on the inelasticity $y=Q^{2} /(s x)$ of the process.
$F_{L}$ is proportional to the cross section for probing the proton with a longitudinally polarized virtual photon and vanishes in the naive Quark Parton Model due to helicity conservation. Starting from $\mathcal{O}\left(\alpha_{s}\right)$, the longitudinal structure function differs from zero, receiving contributions from both quarks and gluons.

At low $x$, the gluon contribution due to photon-gluon fusion greatly exceeds the quark contribution. Therefore, measuring $F_{L}$ provides a rather direct way of studying the gluon density and QCD dynamics at small $x$, i.e., the transition to the high parton density regime. Measurements can be used to test several phenomenological and QCD models describing the low $x$ behavior of the DIS cross section, including color dipole models [83, 84, 85] and expectations from DGLAP fits performed at NLO and NNLO accuracy of QCD. Possible deviations from the DGLAP behavior in the small $x$, low $Q^{2}$ region can be studied by varying kinematic cuts to the data used in the fits.

The longitudinal structure function, or the equivalent cross section ratio $R=\sigma_{L} / \sigma_{T}=$ $F_{L} /\left(F_{2}-F_{L}\right)$, was first measured in fixed target experiments and found to be small at large $x, x \geq 0.01$, see, e.g., Ref. [86]. H1 [30] and ZEUS [87] have recently combined their measurements of $\sigma_{r}$ for three different proton beam energies [20], $E_{p}=920,575$, and 460 GeV , see Fig 1.5 in Sec. 1.3. The extracted $F_{L}$, shown in Fig. 1.12, covers a wide kinematic range, spanning $2.5<Q^{2}<800 \mathrm{GeV}^{2}$ and $0.0006<x<0.0036$. As can be seen, $F_{L}$ is clearly non-zero, and there is some mild tension with the HERAPDF1.0 fit based on DGLAP evolution [20] at the lowest values of $x$ and $Q^{2}$ where one expects non-linear effects to be relevant; see Chapter 5 on $e A$ physics. In this regime, predictions from the dipole model provide a better description of the data. However, the achieved statistical precision of the combined H1 and ZEUS measurement is too limited to be conclusive.

### 1.6.2 Measurement Strategy and Experimental Challenges

The measurement of $F_{L}$ relies on an accurate determination of the variation of the reduced cross section (1.6) for common values of the ( $x, Q^{2}$ ) bin centers at different beam energies, i.e., c.m.s. energies $\sqrt{s}$. Relative normalizations and systematic uncertainties of the different data sets for $\sigma_{r}$ have to be well under control.
$F_{L}$ and $F_{2}$ can be extracted simultaneously from $\sigma_{r}$ by plotting $\sigma_{r}$ for fixed values of $\left(x, Q^{2}\right)$ as a function of $y^{2} / Y_{+} . F_{L}$ is then determined as the slope of the line fitted to the measurements of $\sigma_{r}$ for different values of $\sqrt{s}: F_{L}\left(x, Q^{2}\right)=-\partial \sigma_{r}\left(x, Q^{2}, y\right) / \partial\left(y^{2} / Y_{+}\right)$. Likewise, $F_{2}$ is the intercept of the fitted line with the $y$ axis: $F_{2}\left(x, Q^{2}\right)=\sigma_{r}\left(x, Q^{2}, y=0\right)$. All measurements at HERA are observed to be consistent with the expected linear dependence [30, 87, 20]. At any given value of $Q^{2}$, the lowest possible $x$ values are only accessed by


Figure 1.12. Combined H1 and ZEUS extraction of $F_{L}$ [20] as a function of $Q^{2}$ averaged over $x$ compared to the HERAPDF1.0 fit and predictions from dipole models.
the highest $\sqrt{s}$, and the slope related to $F_{L}$ cannot be determined. Hence, the Rosenbluth separation limits the kinematic coverage of $F_{L}$ at small $x$. At larger values of $x$, measurements of $\sigma_{r}$ for various different $\sqrt{s}$ are available and the slopes can be straightforwardly extracted.

The contribution of $F_{L}$ to the reduced cross section (1.6) can be sizable only at large values of $y$. For low values of $y, \sigma_{r}$ is very well approximated by the structure function $F_{2}$ [30, 87, 20. Low $y$ data can be used to normalize data sets taken at different c.m.s. energies relative to each other. For measurements at high $y$ the reconstruction of the DIS kinematics using the scattered lepton, the so called "electron method", has the best resolution and was used at HERA.

In the large $y$ region, $y \gtrsim 0.5$, and low $x$ the electron method is prone to large QED radiative corrections which can reach a level of more than $50 \%$ of the Born cross section. Studies based on the DJANGO [88] and HECTOR [89] programs for HERA kinematics show that the largest radiative contributions arise because of hard initial-state radiation (ISR) from the incoming lepton [30]. The radiated photon usually escapes in the beam pipe and the $E-P_{z}$ of the event is reduced. Therefore, hard ISR can be efficiently suppressed to a level of about $10 \%$ at HERA with only a slight residual dependence on $y$ by requiring $E-P_{z}$ close to the nominal value of twice the electron beam energy implied by energymomentum conservation [30]. $E-P_{z}$ can be reconstructed from the measured final-state particles. At the highest $y, y \gtrsim 0.7$, corrections increase due to QED Compton events which can be rejected by certain topological cuts. All cross section measurements at HERA are corrected for QED radiation up to $\mathcal{O}\left(\alpha_{e m}\right)$ using HERACLES [90] which is included in the DJANGOH package; further details can be found in Sec. 7.3,

Kinematically, for low $Q^{2}$, large values of $y$ correspond to low energies of the scattered lepton. Selecting high $y$ events is thus further complicated due to a possibly large background from energy deposits of hadronic final state particles leading to fake electron signals. However, the cut on $E-P_{z}$ also suppresses such type of backgrounds. In addition, electron tracking, which is foreseen for an EIC detector, will largely eliminate fake electron signals as an additional cut on $E / p \simeq 1$ can be placed to identify the lepton.

Extractions of $F_{L}$ are certainly the most demanding inclusive structure function measurements but an EIC will have many advantages compared to HERA, in particular, the possibility to vary $\sqrt{s}$ in a wide range for high luminosity collisions. Also, much better detector capabilities, for instance, concerning the electron, are foreseen. One can also take


Figure 1.13. Projected uncertainties for an extraction of $F_{2}$ and $F_{L}$ from a Rosenbluth separation for data taken at three different c.m.s. energies. Also shown are theoretical expectations at NNLO based on the ABKM09 set of PDFs [19] (see text).
advantage of all the analysis techniques and Monte Carlo codes developed for HERA to deal with QED radiative corrections.

### 1.6.3 Expectations for the EIC

Pseudo-data for the reduced cross section (1.6) have been generated using the Monte Carlo generator LEPTO 91 for the first stage of an EIC ( 5 GeV electrons on 100, 250, and 325 GeV protons). The CTEQ6L set of PDFs 82 has been used in the simulations. The hadronic final state was simulated using JETSET [81]. We note that the current pseudo-data do not include any simulations of QED radiative effects and reflect statistical uncertainties which could be achieved by running one month at each of the beam energy settings with the projected luminosities for eRHIC. In addition, a $1 \%$ systematic uncertainty is added.

Figure 1.13 shows the structure functions $F_{L}$ and $F_{2}$ extracted from the pseudo-data of the reduced cross section by means of a Rosenbluth separation, requiring a minimum scattered lepton momentum of $0.5 \mathrm{GeV}, Q^{2}>1 \mathrm{GeV}^{2}, 0.01<y<0.90$, and $0.5^{\circ}<\theta<$ $179.5^{\circ}$. To guide the eye, the expected uncertainties are placed on theoretical expectations for $F_{2, L}$ at NNLO accuracy using the ABKM09 set of PDFs [19]. One should note that these PDFs use only data with $Q^{2}>2.5 \mathrm{GeV}^{2}$ in their fit and, hence, the behavior of $F_{2, L}$ in the lowest $Q^{2}$ bin must be taken with a grain of salt and are only for illustration. The extracted uncertainties take detector smearing of the scattered electron momentum into account. The momentum resolution was taken from ZEUS, i.e., $\delta p / p=0.85 \%+0.25 \% \times p$.

### 1.6.4 Summary and To-Do Items

Like for most inclusive and semi-inclusive measurements at the EIC, an extraction of $F_{L}$ will be dominated by systematic uncertainties which need to be thoroughly addressed. This is work in progress. It is planned to study the unfolding of $F_{L}$ in great detail both in $e p$ and $e A$ scattering, including QED radiative corrections and a full simulation of the detector. This will elucidate to what extent the methods developed and used at HERA [30, 87, 20] are suited for high precision measurements of $F_{L}$ aimed at the EIC. In any case, it will be crucial to design the relevant detector components very carefully to optimize

- the luminosity measurement and its relative calibration for running at different c.m.s. energies,
- the lowest lepton momentum we can detect ( 0.5 GeV would be desirable),
- the identification of the scattered lepton to suppress potential background from misidentified hadrons,
- the resolution in momentum and scattering angle of the scattered lepton, and
- the acceptance for the hadronic final state to suppress events which have a photon radiated from the incoming or outgoing lepton as well as quasi real photo-production events.

Details on the design of the detector are given in Sec. 7.3. Also, it will be possible to extract $\mathrm{F}_{L}$ from the EIC data alone, but the combination of the EIC reduced cross section measurements with the ones from HERA may provide an even better lever arm in a larger $x, Q^{2}$ range. This needs to be investigated.

Finally, we note that even for statistically very precise measurements of $\sigma_{r}$, the Rosenbluth separation of $F_{L}$, i.e., the determination of the slope with respect to $y^{2} / Y_{+}$, can lead to significantly larger uncertainties if the measured values of $\sigma_{r}$ have very similar $y^{2} / Y_{+}$. This source of uncertainties needs be minimized by optimizing the binning in $y$ and the set of different c.m.s. energies $\sqrt{s}$. Studies is this direction are ongoing as well.

### 1.7 Theoretical status of inclusive heavy quark production in DIS

Sergey Alekhin, Johannes Blümlein, Sven-Olaf Moch

### 1.7.1 Introduction

Heavy quark production gives a sizable contribution to the unpolarized DIS structure functions at small $x$, see, e.g., [92, 93, 94, 95]. For the foreseen EIC kinematics of DIS it yields up to $10 \%$ of the inclusive cross section. Therefore in order to employ the full potential of the small- $x$ EIC data for phenomenology one has to provide an accurate theoretical description of heavy-quark electro-production within perturbative QCD.

For the light-parton contributions to DIS structure functions a theoretical accuracy of $O$ (few \%) is achieved, with the complete QCD corrections up to 3-loops being available, see also Sec. 1.2, In the case of the fixed-flavor-number scheme (FFNS) the heavy flavor corrections are available only to $O\left(\alpha_{s}^{2}\right)$. This can be a bottleneck for the analysis of high-precision data. Therefore, progress in the higher-order calculations of heavy-quarkproduction coefficient functions is quite important for the EIC phenomenology. For the variable-flavor-number scheme (VFNS) the massive quarks are considered on the same footing as the massless ones. Furthermore, the heavy-quark PDFs appearing in the VFNS are derived from the light-parton PDFs and the appropriate massive operator-matrix elements (OMEs). The VFNS coefficient functions are known up to 3-loop accuracy due but the massive OMEs are only available to the NLO corrections. This limits the theoretical accuracy of the VFNS as well.

In the following we summarize the state-of-art in calculations of the NNLO corrections to the unpolarized heavy-quark coefficient functions and to the massive OMEs. The FFNS and VFNS are compared to the available HERA data and to each other. We also discuss the implementation of the running-mass scheme for the NLO and NNLO heavy-quark coefficient functions and the resulting improvement in the perturbative stability related to this definition.

### 1.7.2 General framework

The heavy flavor corrections to deep-inelastic structure functions emerge in the Wilson coefficients for the respective processes, i.e., they contribute in terms of virtual and final state effects. Heavy quarks have no strict partonic interpretation since partons are massless, and by virtue of this, infinitely long lived, with the possibility to move collinear to each other. Adopting this picture, heavy quarks can be singly or pair produced from massless partons and the gauge bosons of the Standard Model as final states. This description is called FFNS, which is the genuine scheme in any quantum-field theoretic calculation. The DIS structure functions $F_{i}\left(x, Q^{2}\right)$ obey the representation

$$
\begin{equation*}
F_{i}\left(x, Q^{2}\right)=\left[\sum_{k=q_{l, g}}\left[C_{i, \text { light }}^{k}\left(x, Q^{2} / \mu^{2}\right)+C_{i, \text { heavy }}^{k}\left(x, Q^{2} / \mu^{2}, m_{h}^{2} / \mu^{2}\right)\right] \otimes f^{k}\left(\mu^{2}\right)\right](x), \tag{1.7}
\end{equation*}
$$

where $q_{l}$ and $g$ label the massless quarks and gluons, $f^{k}\left(\mu^{2}\right)$ are the PDFs, $C_{i, \text { light(heavy }}^{k}$ the massless (massive) Wilson coefficients, $h=c, b$ the charm and bottom quarks, and $\otimes$ denotes the Mellin convolution. Other approaches derive from this description.

In case of unpolarized DIS the LO contributions were given in [96, 97, 98, 99] and the NLO corrections were calculated in semi-analytic form in [100, 101]. For asymptotic values $Q^{2} \gg m_{h}^{2}$ one may obtain the massive Wilson coefficients in analytic form. This is due to a factorization theorem [102] relating the massive Wilson coefficients $C_{i, \text { heavy }}^{k}$ to universal massive OMEs and the massless Wilson coefficients [77, 6, 103, 10]. As comparisons up to NLO showed [102], these representations are valid for the structure function $F_{2}\left(x, Q^{2}\right)$ if $Q^{2} / m_{h}^{2} \gtrsim 10$. To $O\left(\alpha_{s}^{2}\right)$ the Wilson coefficients were obtained in [102, 104, 105] at general values of the Mellin variable $N$. A first contribution to the 3-loop corrections was given in [106] by the $O\left(\alpha_{s}^{2} \varepsilon\right)$ terms which contribute to the logarithmic terms $O\left(\ln ^{k}\left(Q^{2} / m_{h}^{2}\right)\right), k=$ $1,2,3$, in $O\left(\alpha_{s}^{3}\right)$. A large number of even Mellin-moments for all unpolarized 3-loop massive OMEs have been calculated in [107] up to $N=10 \ldots 14$ depending on the respective channel. For the structure function $F_{L}\left(x, Q^{2}\right)$ the asymptotic 3-loop corrections were given in [108] for general values of $N$. However, they are valid at $1 \%$ accuracy at much higher scales of $Q^{2} / m_{h}^{2} \gtrsim 800$ only. All logarithmic terms at $O\left(\alpha_{s}^{3}\right)$ for the heavy flavor Wilson coefficients contributing to the structure function $F_{2}\left(x, Q^{2}\right)$ are known [109, 110]. More than this, all the contributions to the constant terms emerging from lower order contributions by renormalization have been calculated, cf. 107] for details. Due to the size of the constant contributions phenomenological applications for the kinematic range available at HERA and the EIC cannot be based on only the logarithmic contributions. QCD corrections to charged current heavy flavor production have been considered in [111, 112, 113 .

### 1.7.3 FFNS and VFNS

The logarithmic contributions in the heavy flavor Wilson coefficients $\propto \ln ^{k}\left(Q^{2} / m_{h}^{2}\right)$ never become large enough in the kinematic region of HERA or the EIC that their resummation would be required [114]. Nonetheless one may introduce a description changing the number of light flavors effectively, which refers to the universal contributions to the heavy flavor Wilson coefficients, consisting of the twist-2 parton densities and the massive OMEs [115, 107, 116, 117. This requires the knowledge of also the gluonic OMEs to 3-loop order [107].

By matching at typical scales $\mu_{f}$ one performs the transition from $n_{f}$ to $n_{f}+1$ massless flavors using the asymptotic relations. In this way one may introduce a heavy quark density. The corresponding representation, which is obtained in terms of a reformulation of the FFNS, is called zero mass variable flavor number scheme (ZMVFNS). It is unique up to the choice of the matching point(s). An important issue is the choice of the scale $\mu_{f}$, for which very often $\mu_{f} \simeq m_{h}$ is used. In Ref. [118] it was shown, however, comparing exact and flavor number matched calculations that this scale is process dependent and often very different scales have to be chosen. In this context various problems arise. Because of the value of the charm to bottom mass ratio, $m_{c}^{2} / m_{b}^{2} \sim 1 / 9$, power corrections due to $m_{c}^{2}$ usually cannot be neglected at scales $\mu^{2} \simeq m_{b}^{2}$. Therefore, sequential decoupling of both charm and bottom quarks is problematic. Furthermore, starting at $O\left(\alpha_{s}^{3}\right)$, Feynman diagrams with both bottom and charm quarks contribute, which cannot be attributed to either the charm or the bottom quark PDF [119. The description of the FFNS, on the other hand, is still possible. Therefore, representations based on the ZMVFNS remain approximations to which one may refer for specific applications. Furthermore, it applies only for the asymptotic case $Q^{2} \gg m_{h}^{2}$.

For the description of data one would like to have a smooth description of the structure


Figure 1.14. Comparison of $F_{2}^{c}$ computed in different schemes to H1 and ZEUS data: GMVFNS in the BMSN prescription (solid lines), 3-flavor scheme (dot-dashed lines), and 4-flavor scheme (dashed lines). The vertical dotted line denotes the position of $m_{c}=1.43 \mathrm{GeV}$. Taken from Ref. [19].
functions at both large and low values of $Q^{2}$, which is called the general mass variable flavor number scheme (GMVFNS). Here, a smooth interpolation is provided by the BMSN scheme [116, 19] given by

$$
\begin{equation*}
F_{2}^{h, \mathrm{BMSN}}\left(n_{f}+1\right)=F_{2}^{h, \text { exact }}\left(n_{f}\right)+F_{2}^{h, \mathrm{ZMVFNS}}\left(n_{f}+1\right)-F_{2}^{h, \text {,asymp }}\left(n_{f}\right), \tag{1.8}
\end{equation*}
$$

where exact corresponds to [100, 101], asymp to its asymptotic form for $Q^{2} \gg m_{h}^{2}$, and ZMVFNS to the value in the zero mass variable flavor scheme. In Fig. 1.14 the transition is shown for values of $x$ between 0.00018 and 0.03 for the kinematics at HERA according to (1.8) (see Ref. [120] for phenomenological variants of the GMVFNS).

### 1.7.4 The massive NNLO corrections and the running mass

The radiative corrections to the massive Wilson coefficients are known to be sizable. In particular, near the production threshold $s \simeq 4 m_{h}^{2}$, where large Sudakov double logarithms $\alpha_{s}^{k} \ln ^{2 k}\left(1-4 m_{h}^{2} / s\right)$ dominate at each order, one may wish to apply resummations; see Refs. [121, 122, 123] for details.

Another aspect at higher orders concerns the definition of the heavy quark mass, since it is a scheme dependent quantity. It is of particular interest to investigate which choice of scheme leads to the best convergence of the perturbative series. Upon conversion of the conventionally used on-shell (pole) mass for heavy quark DIS to the running mass $m_{h}(\mu)$ in the $\overline{\mathrm{MS}}$-scheme, one observes a considerable improvement of scale stability and convergence of the perturbative expansion. The latter aspect is demonstrated in Fig. 1.15, Here one uses the Wilson coefficients to NLO and refers to the approximate result valid in the threshold region [121, 122, 123 to give an estimate for the NNLO value, see Ref. [124].


Figure 1.15. The mass dependence of $F_{2}^{c}$ for $Q^{2}=10 \mathrm{GeV}^{2}, x=10^{-3}$, and $\mu_{r}=\mu_{f}=\sqrt{Q^{2}+4 m_{c}^{2}}$ using the PDFs of [19. $m_{c}$ is taken in the on-shell scheme (left) and in the $\overline{\mathrm{MS}}$ scheme (right) at LO (blue), NLO (green), and $\mathrm{NNLO}_{\text {approx }}$ (red); from Ref. [124].


Figure 1.16. The combined HERA data on $F_{2}^{c}$ in comparison with the prediction of a fit 124 performed in the running-mass scheme 125 .


Figure 1.17. The 1- $\sigma$ error bands (shaded area) for our NNLO 4-flavor (left panel) and 5 -flavor (central and right panels) $s, c$, and $b$ quark distributions in comparison to the corresponding MSTW2008 NNLO PDFs [22] (dashed lines); from Ref. 19].

The phenomenological impact of the mass scheme re-definition was checked for the ABKM fit of Ref. [19]. In a variant of this fit [124] the heavy-quark electro-production was considered in the running mass scheme and with the approximate NNLO corrections taken into account. $m_{c}$ was fitted to the DIS data simultaneously with the PDG world average [3] added to the fit as an additional constraint. In this way the value of $m_{c}\left(m_{c}\right)=$ $1.18 \pm 0.06 \mathrm{GeV}$ was obtained. The corresponding predictions for the semi-inclusive structure function $F_{2}^{c \bar{c}}$ are in good agreement with the preliminary HERA data in a wide kinematical region, cf. Fig. 1.16. This result gives an additional justification of the validity of the FFNS up to $Q^{2} \sim 1000 \mathrm{GeV}^{2}$, i.e., in the entire kinematic range relevant for an EIC.

### 1.7.5 Heavy-flavor PDFs

For applications at high-energy hadron colliders, schemes with 4- and 5-light flavors need to be considered. The necessary charm- and bottom PDFs are generated perturbatively. In Fig. 1.17 the results for the $s, c$, and $b$ quark flavors are shown at NNLO accuracy as determined in two global fits to the world data [19, 22]. The 1- $\sigma$ error bands correspond to the analysis of [19]. The central values of the MSTW08 distributions turn out to lie below those found in the ABKM09 analysis for the $c$ and $b$ quark distributions in the whole kinematic range of HERA due to the smaller gluon density [22]. The strange quark distribution still exhibits large errors; see also Sec. 1.5. Measurements at the EIC are expected to considerably improve both the strange and charm quark densities thanks to the much higher luminosities than at HERA.

## $1.8 \quad F_{2, L}$ (charm) at an EIC

Elke C. Aschenauer, Marco Stratmann

Section 1.7 gave an outline of the theoretical status of heavy flavor contributions to DIS structure function and a comparison to HERA data. The mass $m_{h}$ of the heavy quark introduces extra theoretical complications including the need for a smooth prescription to cover both the threshold ( $Q \simeq m_{h}$ ) and the asymptotic ( $Q \gg m_{h}$ ) region, the scheme used for $m_{h}$ (on-shell or $\overline{\mathrm{MS}}$ ), and the actual value of $m_{h}$ used in the calculations.

Detailed experimental results from the EIC, in particular, for the so far unmeasured charm contribution to $F_{L}$, will help to refine the current theoretical understanding. In the entire kinematic domain of the EIC one expects the FFNS to be applicable for $F_{2}^{c}$; see Sec. 1.7. Differences between the exact, massive FFNS results, and the ZMVFNS are expected to be much more pronounced for $F_{L}^{c}$, see, e.g., Fig. 7 in [114], than for $F_{2}^{c}$ shown in Fig. 1.14.

The extraction of $F_{L}^{c}$ requires a Rosenbluth separation and should proceed along very similar lines as discussed already in Sec. 1.6. The extra experimental complication is the requirement to detect a charm quark in the final state. A quantitative feasibility study is still ongoing. We note that the detection of charmed mesons is important also for other physics topics. Therefore the design of the detector foresees to have particle identification for pions and kaons to fully reconstruct charmed mesons via their $K \pi$ decay channel. In addition, a micro-vertex detector is expected to provide a vertex resolution of $5 \mu \mathrm{~m}$ to separate charmed mesons from B- and other mesons by measuring a displaced decay vertex. Using such techniques for a measurement of $F_{L}$ requires to detect a second decay lepton with a displaced vertex in addition to the scattered lepton. This, together with good lepton identification, should provide a high charmed meson detection efficiency. The required luminosities for a precise measurement of $F_{2, L}^{c}$ will scale with the achieved charm detection efficiency of the EIC detectors and the smaller reduced cross section for charm as compared to the fully inclusive $\sigma_{r}$ studied in Sec. [1.6. To illustrate the relative size of $F_{L}^{c}$ and $F_{2}^{c}$ we present in Fig. 1.18 some theoretical expectations at NLO accuracy based on the ABKM set of PDFs [19] see Sec. 1.7 for details.


Figure 1.18. Expectations for $F_{2, L}^{c}\left(x, Q^{2}\right)$ in bins of $Q^{2}$ using the ABKM set of PDFs [19].

### 1.9 Probing intrinsic charm at the EIC

Marco Guzzi, Pavel Nadolsky, Fredrick Olness

In the variable flavor number (VFN) factorization scheme [126, 127, 68, heavy quark flavors are actively included in the PDF evolution via gluon splitting to a heavy quark pair $g \rightarrow Q \bar{Q}$. While the heavy quark PDF $f_{Q}(x, \mu)$ is often taken to vanish below the mass threshold $\left(\mu<m_{Q}\right)$, there is the possibility that the proton contains non-vanishing heavy quark constituents even for scales below $m_{Q}$; this component of the heavy quark PDF is identified as the intrinsic parton distribution [56, [57, 128, 129], in contrast to the extrinsic distribution generated by gluon splitting $g \rightarrow Q \bar{Q}$.

While we can introduce intrinsic parton distributions for both charm and bottom quarks, we will focus here on the intrinsic charm (IC). Operationally, the total charm PDF is then composed as $f_{c}(x, \mu)=f_{c}^{e x t}(x, \mu)+f_{c}^{\text {int }}(x, \mu)$. For the extrinsic component, we generally take the boundary condition $f_{c}^{e x t}(x, \mu)=0$ for $\mu<m_{c}$, i.e., we do not need to assume an initial functional form for $f_{c}^{e x t}$, as it is determined purely by the gluon evolution.

Conversely, for the IC component $f_{c}^{\text {int }}$ we do need to assume a functional form. Here, we consider two typical shapes of $f_{c}^{i n t}$ at the initial scale $\mu=m_{c}$, assuming $m_{c}=1.3 \mathrm{GeV}$.

- In the BHPS model [56, 57, 130, the intrinsic charm is concentrated at large $x$.
- In sea-like models [129], the intrinsic charm is spread over all $x$ values.

Sample distributions of IC PDFs were obtained in a global QCD fit of hadronic data [129. We display them in Fig. [1.19] In these models, the momentum fraction carried by the charm can be varied in some range. Roughly, an intrinsic momentum fraction of $2 \%$ or $3 \%$ is at the outer limit of what is allowed in the context of a global fit.


Figure 1.19. Left, middle: charm PDFs for the BHPS model, at $\mu=2$ and 100 GeV . The upper dashed curve is for a momentum fraction of $2 \%$, and the lower for $0.57 \%$. The shaded band is the CTEQ6.5 PDF uncertainty. Right: charm PDFs for the sea-like model. The upper curve is for a momentum fraction of $2.4 \%$, and the lower for $1.1 \%$. Figs. are taken from [129.

For heavy quark production in the threshold region $\left(\mu \sim m_{Q}\right)$, the magnitude of the intrinsic component will be large on the relative scale compared to the extrinsic contribution. At higher $\mu$ scales, the DGLAP evolution will increase the extrinsic component via $g \rightarrow Q \bar{Q}$ splitting. However, the distinctive shape of the BHPS distribution, with its characteristic large- $x$ enhancement, remains clearly evident even at much higher scales $\mu \gg m_{c}$.

We now consider two different c.m.s. energies for an EIC [131] and investigate the degree to which one can distinguish the IC component based on measurements of the charm


Figure 1.20. Charm contribution to the reduced NC $e^{-} p$ DIS cross section at $\sqrt{s}=45$ and 105 GeV . For each IC model, curves for charm momentum fractions of $1 \%$ and $3.5 \%$ are shown. For comparison we display the number of events $d N_{e} / d x$ for $10 \mathrm{fb}^{-1}$, assuming perfect charm tagging efficiency.
contribution to the DIS cross section. Alternatively, the IC can be searched for by measuring the longitudinal structure function $F_{L}$ or angular distributions [132]. In Fig. 1.20 we display the reduced cross section $\sigma_{r, c}$ for semi-inclusive DIS charm production at an EIC. The reduced charm cross section is defined as in Eq. (1.6). The probed ranges of $y$ are displayed in the figures.

The number of events for a conservative integrated luminosity $\mathcal{L}=10 \mathrm{fb}^{-1}$ has been computed as $d N_{e} / d x=\mathcal{L}\left\langle d \sigma_{c} / d x\right\rangle$ where $\left\langle d \sigma_{c} / d x\right\rangle$ is the average cross section in a $Q$ bin of size 0.15 GeV , evaluated at NLO accuracy. The shaded band represents the error on the cross section induced by the CTEQ6.6 PDF uncertainty 43.

For both BHPS and sea-like IC, we observe that the cross sections significantly exceed the nominal CTEQ6.6 values. While a momentum fraction of $3.5 \%$ is easily distinguished, even the intrinsic charm models with $1 \%$ can be resolved with moderate integrated luminosities.

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We appreciate a discussion with J. Pumplin.

# 1.10 Status of helicity-dependent PDFs and open questions to be addressed at an EIC 

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### 1.10.1 Introduction

Helicity-dependent or polarized PDFs (pPDFs) tell us precisely how much quarks and gluons with a given momentum fraction $x$ tend to have their spins aligned with the spin direction of a nucleon in a helicity eigenstate. Their knowledge is essential in the quest to answer one of the most basic and fundamental questions in hadronic physics, namely how the spin of a nucleon is composed of the spins and orbital angular momenta of its constituents.

The nucleon spin structure can be best understood in high-energy scattering experiments where quarks and gluons behave as almost free particles at scales $\mu>\Lambda_{Q C D}$. The relevance of pPDFs or research in spin physics in general is reflected in more than a dozen vigorous experimental programs in the wake of the unexpected finding that only very little of the proton spin is actually carried by its three valence quarks almost twenty-five years ago. The experiments have measured with increasing precision various observables sensitive to different combinations of quark and gluon polarizations in the nucleon. This progress was matched by advancements in corresponding theoretical higher order calculations in the framework of pQCD and phenomenological analyses of available data. Potentially large sea quark and/or gluon polarizations were initially thought to be ways to account for the "missing" proton spin, but at the same time, both turned out to be challenging to access experimentally.

The most comprehensive global fits include all available data taken in spin-dependent DIS, semi-inclusive DIS (SIDIS) with identified pions and kaons, and proton-proton collisions. They allow for extracting sets of pPDFs consistently at NLO accuracy along with estimates of their uncertainties [25, 26]. Contributions from the orbital angular momenta of quarks and gluons completely decouple from such type of experimental probes and need to be quantified by other means. Here, transverse momentum-dependent PDFs or generalized PDFs appear to be the most promising approaches which will be discussed elsewhere in Chapters 2 and 3, respectively.

Despite the impressive progress made in the past couple of years both experimentally and theoretically many fundamental questions related to the proton's helicity structure still remain unanswered and shall be summarized below; addressing them and providing answers is a prime target for an EIC.

Present fixed-target experiments suffer from their very limited kinematic coverage in $x$ and $Q^{2}$, which is insufficient to precisely study, for instance, QCD scaling violations for the polarized DIS structure function $g_{1}\left(x, Q^{2}\right)$ which in turn can be linked to the $x$ dependence of the polarized gluon density $\Delta g(x)$. There are numerous other opportunities for an EIC to further our understanding of the nucleon spin structure which will be listed below and discussed in some details in Secs. 1.11, 1.12, and 1.13,

### 1.10.2 Current status of global pPDF fits - baseline for EIC projections

Unlike unpolarized PDF fits, where a separation of different quark flavors is obtained from inclusive DIS data taken with neutrino beams, differences in polarized quark and


Figure 1.21. COMPASS results [133, 134 for SIDIS spin asymmetries on a deuteron (left) and proton target (right) compared to DSSV and DSSV + fits (see text).
antiquark densities are at present determined exclusively from SIDIS data and hence require knowledge of fragmentation functions. Recently published SIDIS data from the COMPASS collaboration [133, 134] extend the coverage in $x$ down to about $x \simeq 5 \times 10^{-3}$, almost an order of magnitude lower than the kinematic reach of the HERMES data used in the DSSV global analysis of 2008 [25, 26]. For the first time, the new results comprise measurements of identified pions and kaons in the final state taken with a longitudinally polarized proton target. Clearly, these data can have a significant impact on fits of pPDFs and estimates of their uncertainties.

In particular, the COMPASS kaon data will serve as an important check of the validity of the strangeness density obtained in the DSSV analysis, which instead of favoring a negative polarization as in most fits based exclusively on DIS data, prefers a vanishing or perhaps even slightly positive $\Delta s$ in the measured range of $x$. One reason for concern is the dependence on fragmentation functions. Even though pion fragmentation functions are rather well constrained [74] by data, kaon fragmentation functions suffer from much larger uncertainties, and this could explain the unexpected result for $\Delta s$ obtained in the DSSV analysis.

Figure 1.21 shows a comparison between the new SIDIS spin asymmetries from COMPASS [133, 134 and the DSSV fit of 2008 [25, 26]. Also shown is the result of re-analysis at NLO accuracy based on the updated data set. This fit, henceforth called "DSSV+", will serve as baseline pPDFs when quantifying the potential impact of projected EIC data on our knowledge of the nucleon spin structure in Sec. 1.11. The differences between the original and the updated fit are hard to notice for both identified pions and kaons. In terms of $\chi^{2}$ values, the original DSSV analysis amounts to 392 units for the original set of 467 data points used in the fit [74]. Adding both deuteron and proton data from COMPASS (88 points) it goes up to 456 and drops by about 4 units upon refitting (DSSV+), which is not really a significant improvement for a PDF analysis in view of non-Gaussian theoretical uncertainties. Recall that in the DSSV analysis a $\Delta \chi^{2} \simeq 9$ (corresponding to $\Delta \chi^{2} / \chi^{2}=2 \%$ ) was tolerated as a faithful, albeit conservative estimate of PDF uncertainties.

In Fig. 1.22 we compare the individual sea quark densities obtained in the original and


Figure 1.22. DSSV and DSSV + sea quark pPDFs and uncertainty bands at $Q^{2}=10 \mathrm{GeV}^{2}$. Also shown is $\Delta g$. The vertical lines indicate the $x$ region constrained by RHIC $p p$ data.
updated DSSV analyses. As can be seen, except for $\Delta s$, the new central fits fall well within the $\Delta \chi^{2}=1$ uncertainty bands of DSSV. The gluon distribution is hardly affected by the new SIDIS data. For DSSV+ we only give the new uncertainty bands (dashed lines) referring to the $\Delta \chi^{2} / \chi^{2}=2 \%$ tolerance criterion.

Although it may seem that the new SIDIS data have little impact on the fit, this is not the case if one studies individual $\chi^{2}$ profiles in more detail. Figure 1.23 shows the contributions to $\Delta \chi^{2}$ from various data sets against variations of the truncated first moments for $\Delta \bar{u}$ and $\Delta \bar{d}$ in the range $0.001 \leq x \leq 1$. Compared to the original DSSV fit one notices a trend towards smaller net polarization as the best fit values shift towards zero. This is induced by the new COMPASS SIDIS data. Both pions and kaons pull in the same direction and to a common smaller best fit value. There is, however, some mild tension with older SIDIS sets, but this is well within the tolerance of the fit and most likely caused by the different $x$ ranges covered by the different data sets. In addition, one finds a significant reduction in the uncertainties, as determined by the width of the $\chi^{2}$ profiles at a given $\Delta \chi^{2}$.

A much debated feature of the strangeness pPDF obtained in the DSSV fit is its unexpected small value at medium-to-large $x$ which, when combined with a node at intermediate $x$, still allows for acquiring a significant negative first moment at small $x$, in accordance with expectations from $\mathrm{SU}(3)$ symmetry (hyperon decay constants $F$ and $D$ ) and fits to DIS data only (see, e.g., Ref. [23]). To investigate the possibility of a node in $\Delta s(x)$ further we present in Fig. 1.24 the $\chi^{2}$ profiles for two different intervals in $x$ : $0.001 \leq x \leq 0.02$ and $0.02 \leq x \leq 1$. Again, the new COMPASS SIDIS data have quite some impact on the profiles but the central value for the combined range, $0.001 \leq x \leq 1$, does not shift from its original DSSV value.

The profiles in Fig. 1.24 clearly show that for $0.001 \leq x \leq 0.02$ the result for $\Delta s$ is a compromise between DIS and SIDIS data, the latter favoring much less negative values.


Figure 1.23. $\chi^{2}$ profiles for the first moments of $\Delta \bar{u}$ and $\Delta \bar{d}$ truncated to $0.001 \leq x \leq 1$.


Figure 1.24. $\chi^{2}$ profiles for the truncated first moment of $\Delta s$ in two different $x$ intervals.

For $0.02 \leq x \leq 1$ everything is determined by SIDIS data and all sets consistently ask for a small, slightly positive strange quark polarization. There is no hint of a tension with DIS data as they do not provide a useful constraint at medium-to-large $x$. We note that at low $x$, most SIDIS sets give indifferent results except the new COMPASS data which extend towards the smallest $x$ values so far and actually do show some preference for a slightly negative value for $\Delta s$. This exemplifies the need for measurements at small $x$. Clearly, all current extractions of $\Delta s$ from SIDIS data show a significant dependence on kaon FFs, see, e.g., Ref. [133, 134]. Better determinations of $D^{K}(z)$ are highly desirable, but should be possible with forthcoming data from $B$-factories, DIS multiplicities, and LHC data. We also notice that in the range $x \gtrsim 0.001$ the hyperon decay constants, the so-called $F$ and $D$ values, do not play a significant role in constraining $\Delta s$ as can be deduced from their relative contribution to $\Delta \chi^{2}$ in Fig. 1.24 . Computations of $\mathrm{SU}(3)$ breaking effects in axial current matrix elements [135, 136], and, more recently, also first lattice results for the first moment of $\Delta s+\Delta \bar{s}$ [137] point towards a sizable breaking of $\operatorname{SU}(3)$ symmetry. To study its validity of one needs to probe $\Delta s(x)$ at smaller values of $x$ at an EIC.

An interesting recent development is that the LSS group produced an update of their pPDF fit using for the first time DIS and SIDIS data simultaneously [28]. As in the DSSV analysis they also utilize DSS fragmentation functions [74]. Their functional form is also very similar to the one used in DSSV and DSSV+. As in their previous analyses they carefully include target mass corrections and phenomenological higher twist corrections for inclusive DIS data. Nevertheless, their obtained pPDFs are very similar to the best fit of DSSV shown in Fig. 1.22. Their strange quark polarization also changes sign as in DSSV but is overall slightly smaller in magnitude. LSS finds non negligible higher twist corrections to inclusive DIS data, however, these conclusions are not fully shared by another recent analysis of polarized DIS data [23]. Ref. [23] also provides an extraction of $\alpha_{s}$ from polarized DIS data. There are also interesting first attempts to perform a pPDF analysis based on neural networks [138, 139 similar to successful global fits of unpolarized data [47. This would provide independent estimates of pPDF uncertainties not biased by the choice of a particular functional form.

### 1.10.3 Open Questions

The status of pPDFs outlined above will likely not change much until the time of EIC operations. Most of the remaining, compelling open questions in spin physics related to pPDFs will be still with us and can be only addressed by extending the kinematic coverage to smaller values of $x$; see the items listed below.

Existing experiments, like PHENIX and STAR at RHIC, will continue to add data in the next couple of years. Parity-violating, single-spin asymmetries for $W$ boson production should reach a level where they help to constrain $\Delta u, \Delta \bar{u}, \Delta d$, and $\Delta \bar{d}$ at large $x$, $0.07 \leq x \leq 0.4$ at scales $Q \simeq M_{W}$ much larger than typically probed in SIDIS [140]. Measurements of double spin asymmetries for di-jets in $p p$ collisions at 500 GeV should improve the current constraints on $\Delta g(x)$ and extend them towards somewhat smaller values of $x$. The strangeness polarization is, however, very hard to access in polarized $p p$ collisions. In the future, JLab12 will add very precise DIS data at large $x$. They will allow us to challenge ideas like helicity retention [141, 142 which predict that $\Delta f(x) / f(x) \rightarrow 1$ as $x \rightarrow 1$. Currently, only $\Delta u / u$ exhibits this trend, while $\Delta d / d$ remains negative up to $x \simeq 0.6$.

We expect an EIC to make significant contributions on the following topics:
Polarized gluon density $\boldsymbol{\Delta g}(\mathbf{x})$ : precise data for the DIS structure function $F_{2}$ in a broad kinematic range in $x$ and $Q^{2}$ from HERA provide the world's best and theoretically cleanest constraint on the unpolarized gluon density; see Sec. 1.3. One of the most important results of HERA was to establish the strong rise of the gluon density at small $x$ which could not be anticipated from previous fixed-target results.

Figure 1.25 summarizes the current situation for polarized DIS. The kinematic coverage is limited to the fixed-target regime. There are no data below $x \simeq 0.005$, and the lever-arm in $Q^{2}$ is very limited, in particular, for the smallest $x$ values. As a consequence, $\Delta g(x)$ is basically unconstrained at small $x$ as is reflected in the large uncertainty band shown in Fig. 1.22. There are theoretical arguments that $\Delta g(x) \simeq x g(x)$ at small $x$ [141] but they cannot be verified experimentally due to the lack of data

The fact that current RHIC data favor a very small gluon density in $0.05 \lesssim x \lesssim 0.2$ [25], perhaps with a node, also greatly complicates the determination of the first moment, $\int_{0}^{1} \Delta g\left(x, Q^{2}\right) d x$, which enters in the fundamental proton spin sum rule in its light-cone gauge formulation [143, 144]. Since contributions to the moment largely cancel in the measured $x$ range, the unmeasured small $x$ region may contribute significantly even up to one unit of


Figure 1.25. Scaling violations for the structure function $x g_{1}^{p}$ in bins of $x$. Experimental data are compared to various fits at NLO accuracy. Figure taken from [23].
$\hbar$.
Precise measurements of the structure function $g_{1}\left(x, Q^{2}\right)$ in a wide kinematic range will be a flagship measurement for an EIC. The polarized gluon density is strongly correlated with QCD scaling violations, $d g_{1}\left(x, Q^{2}\right) / d \ln Q^{2} \simeq-\Delta g\left(x, Q^{2}\right)$, i.e., a large positive $\Delta g$ at small $x$ is expected to drive $g_{1}$ towards large negative values for $x \simeq 10^{-(3 \div 4)}$. A precise DIS measurement will also constrain the quark singlet density $\Delta \Sigma\left(x, Q^{2}\right)$ and its first moment, i.e., the total quark spin contribution to the proton spin, much better.

Complete flavor separation: given the significant impact present SIDIS data already have in global analyses of pPDFs, it is easy to imagine that an EIC with its extended kinematic coverage can turn SIDIS measurements into a precision tool for detailed studies of $\Delta u, \Delta \bar{u}, \Delta d, \Delta \bar{d}, \Delta s$, and $\Delta \bar{s}$. For instance, a precise determination of a possible asymmetry in the light quark sea, $\Delta \bar{u}(x)-\Delta \bar{d}(x)$ will challenge expectations from model calculations. Again, current QCD fits have revealed rather complicated functional forms with possible nodes for the quark densities which need to be studied more precisely.

Prerequisites are a detector with excellent particle ID in an as large as possible portion of phase space and an improved theoretical knowledge of FFs, in particular, for kaons. For the latter, significant progress will be made by the time the EIC turns on. In any case, there will be also plenty of opportunities to further constrain them at an EIC if necessary.

Novel electroweak probes in DIS: At large enough $Q^{2}$ and with the envisioned luminosities of up to $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ an EIC has the unique opportunity to access polarized electroweak structure functions via charged and neutral current DIS measurements. These novel probes depend on various combinations of polarized quark PDFs and provide an alternative way of separating different quark flavors for $x \gtrsim 10^{-2}$. Prerequisites are both electron and positron beams to fully exploit charged current (CC) DIS, i.e., the pPDF combinations probed in the exchange of $W^{-}$and $W^{+}$bosons. Also, one needs to be able
to reconstruct $x$ and $Q^{2}$ from the final state hadrons in the absence of a scattered lepton in CC DIS.

Strangeness polarization, $\Delta \mathrm{s}-\Delta \overline{\mathrm{s}}$, and $\mathrm{SU}(3)$ symmetry: As mentioned already, the surprisingly small strangeness density determined from SIDIS data has triggered a lot of discussions recently. It is certainly of outmost importance to precisely map $\Delta s(x)$ and $\Delta \bar{s}(x)$ down to sufficiently small values of $x$ to reliably determine their first moments. If $\mathrm{SU}(3)$ symmetry is approximately valid, one expects a significantly negative first moment for strangeness; if, on the other hand, $\mathrm{SU}(3)$ symmetry is badly broken at a $20 \div 30 \%$ level, $\Delta s(x)$ can remain small and perhaps even slightly positive down to small $x$. Ideas have been put forward that $\Delta s(x)$ and $\Delta \bar{s}(x)$ may have opposite polarizations which could explain the smallness of $\Delta s+\Delta \bar{s}$ in DIS but would result in a potentially sizable $\Delta s-\Delta \bar{s}$.

At an EIC there are different strategies to determine $\Delta s$ and $\Delta \bar{s}$. The most promising one is through SIDIS production of charged kaons. Once $K^{+}$and $K^{-}$yields are known with high precision and uncertainties for kaon FFs are well understood one can attempt an extraction of $\Delta s(x)$ and $\Delta \bar{s}(x)$ in a large range of $x$. Alternatively, one can study charm production in CC DIS with a polarized proton target. If one has electron and positron beams available, the yields of $D$ and $\bar{D}$ mesons should be related to $\Delta s(x)$ and $\Delta \bar{s}(x)$, respectively.

Heavy flavor contributions to $\mathrm{g}_{1}$ : for presently available data, any contribution from heavy quarks, i.e., charm and bottom, can be safely ignored. From HERA we know, however, that at sufficiently small values of $x$ and large enough $Q^{2}$, charm quarks can contribute as much as $20 \div 25 \%$ to a measurement of $F_{2}$. It is important to determine the charm contribution to $g_{1}$ at small $x$ experimentally and to properly include it in future global analyses. Since $g_{1}^{c}$ is mainly driven by photon-gluon-fusion it can be also a viable probe of $\Delta g$ in the small $x$ region.

Bjorken sum rule: the Bjorken sum rule is certainly one of the best known quantities in perturbative QCD. Corrections up to $\mathcal{O}\left(\alpha_{s}^{4}\right)$ have been calculated [32]. There is also a nontrivial connection to Adler's $D\left(Q^{2}\right)$ function defined in $e^{+} e^{-}$annihilation through the generalized Crewther relation [145, 32] involving the QCD $\beta$ function which incorporates the deviation from the limit of exact conformal invariance. It is certainly important and legitimate to ask to what level of precision an EIC can verify this fundamental sum rule.

Since the Bjorken sum rule relates the moments of the $g_{1}$ structure functions for protons and neutrons, it first of all requires an "effective neutron target" such as Helium-3. Perhaps the biggest challenge is then to develop a polarimeter to control its polarization with high accuracy. Most likely this will be the limited factor for a measurement of the Bjorken sum.

In addition, the sum rule involves the first moments of $g_{1}$, i.e., one has to worry about possible extrapolation uncertainties for $x \rightarrow 0$. However, since the Bjorken sum is a nonsinglet quantity, contributions from the small $x$ region should be under control up to a $1 \div 2 \%$ once a measurement down to $x \simeq 10^{-4}$ can be performed. At this level of accuracy one may also expect contributions to matter which break isospin symmetry.

### 1.11 Opportunities in spin physics at an EIC

Elke C. Aschenauer, Rodolfo Sassot, Marco Stratmann

Here, we demonstrate how an EIC can address the fundamental open questions concerning the proton's helicity structure raised in the previous Section. A detailed, quantitative discussion of novel electroweak effects in polarized DIS can be found in Secs. 1.12 and 1.13

### 1.11.1 Scaling violations in inclusive DIS and their impact on $\Delta \mathrm{g}(\mathrm{x})$

A precise determination of the polarized gluon distribution $\Delta g\left(x, Q^{2}\right)$ in a broad kinematic regime is a primary goal for the EIC. Current determinations of $\Delta g$ suffer from both a limited $x$ coverage and fairly large theoretical scale ambiguities in polarized $p p$ collisions for inclusive (di)jet [146, 147] and pion production [148, 149]. Several channels are sensitive to $\Delta g$ in $e p$ scattering at collider energies such as DIS jet [150, (151] or charm [152, 153, 154] production but QCD scaling violations in inclusive polarized DIS have been identified as the golden measurement.

The inclusive structure function $g_{1}\left(x, Q^{2}\right)$ is the most straightforward probe in spin physics and has been determined in various fixed-target experiments at medium-to-large values of $x$ in the last two decades. It is also the best understood quantity from a theoretical point of view. Unlike for most other processes, full NNLO corrections of the relevant hard scattering coefficient functions are available [15], and partial results for the polarized splitting functions at NNLO have been reported in [14] recently. A consistent framework up to NNLO accuracy will be in place by the time of first EIC operations and is required in order to limit the size of residual theoretical scale uncertainties to the anticipated unprecedented level of precision for a polarized DIS experiment. To achieve the latter, systematic uncertainties need to be controlled extremely well which imposes stringent requirements on the detector performance, acceptance, and the design of the interaction region. Necessary, on-going studies comprise the detection of scattered electrons down to small momenta of $\mathcal{O}(0.5 \mathrm{GeV})$ to access small $x$, the required resolution in momentum and angle of the scattered lepton, and the unfolding of QED radiative corrections, see Sec. 7.3,

For studying scaling violations $d g_{1}\left(x, Q^{2}\right) / d \log Q^{2}$ efficiently, it is not only essential to have good precision but also to cover the largest possible range in $Q^{2}$ for any given fixed value of $x$. The accessible range in $Q^{2}$ is again linked (via the inelasticity $y$ ) to the capabilities of detecting electrons in an as wide as possible range of momenta and scattering angles. For a detailed discussion of the kinematic coverage at the EIC see Sec. 7.3,

Figure 1.26 highlights the main motivation for a measurement of $g_{1}$ at the EIC. The significant uncertainty in $\Delta g\left(x, Q^{2}\right)$ at $x \lesssim 0.01$ shown in Fig. 1.22 translates into a large spread of predictions for the behavior of $g_{1}$ at small $x$. The spin-dependent scale evolution is such that $d g_{1}\left(x, Q^{2}\right) / d \log Q^{2}$ at low $x$ is strongly correlated with the negative of $\Delta g\left(x, Q^{2}\right)$, i.e., a positive gluon distribution drives $g_{1}$ at small $x$ to more and more negative values as $Q^{2}$ increases, and vice versa. Hence, a precision measurement of $g_{1}$ and its logarithmic scale dependence will determine $\Delta g\left(x, Q^{2}\right)$ at small $x$, hereby dramatically reducing the extrapolation uncertainties of the integral $\int_{0}^{1} \Delta g\left(x, Q^{2}\right) d x$ entering the proton spin sum rule. Depending on the shape of $\Delta g\left(x, Q^{2}\right)$ in the unmeasured region, it is currently still possible to accommodate up to one unit of $\pm \hbar$ at small $x$ [25, 26], i.e., twice the proton spin! Having determined the functional form of $\Delta g\left(x, Q^{2}\right)$ down to about $10^{-4}$, even extreme extrapolations to $x \rightarrow 0$ are not expected to contribute anymore significantly to the integral


Figure 1.26. Spread of predictions for $g_{1}(x)$ induced by the current uncertainty in $\Delta g(x)$.
$\int_{0}^{1} \Delta g\left(x, Q^{2}\right) d x$.
To quantify the impact of polarized DIS measurements on our knowledge of the gluon density we have performed a series of global QCD analyses based on realistic pseudo-data for various c.m.s. energies at a first stage of eRHIC: 5 GeV electrons on $50,100,250$, and 325 GeV protons. The simulations are based on the PEPSI Monte Carlo code [155] using the GRSV "std" set of polarised PDFs [24]. The statistical precision of the data sets for 100-325 GeV protons corresponds to about two months of running at the anticipated luminosities for eRHIC with an assumed operations efficiency of $50 \%$. For $5 \times 50 \mathrm{GeV}$ an integrated luminosity of $5 \mathrm{fb}^{-1}$ was assumed. Demanding a minimum $Q^{2}$ of $1 \mathrm{GeV}^{2}$, $W^{2}>10 \mathrm{GeV}^{2}$, the depolarization factor of the virtual photon to be $D(y)>0.1$, and $0.1 \leq y \leq 0.95$, the highest $\sqrt{s} \simeq 70 \div 80 \mathrm{GeV}$ allows one to access $x$ values down to about $2 \times 10^{-4}$. As can be seen from the kinematic plots in Sec. 7.3, the lever-arm in $Q^{2}$ more and more diminishes if smaller $x$ values are probed. For instance, choosing $Q_{\text {min }}^{2}=2 \mathrm{GeV}^{2}$ would limit the $x$ range to $x \gtrsim 4 \times 10^{-4}$ at the first stage of eRHIC. Clearly, one wants to utilize $Q^{2}$ values as low as possible in a QCD analysis but once actual EIC data become available one needs to systematically study how far down $Q_{\min }^{2}$ can be pushed before the pQCD framework breaks down. We plan to investigate the impact of the $Q_{\min }^{2}$ cut on constraining $\Delta g$ based on analyses with the pseudo-data. At small enough $x$ one may observe also deviations from standard DGLAP evolution as we will discuss briefly below. A full eRHIC with energies of up to 30 GeV electrons on 325 GeV protons is certainly desirable as it would cover the most interesting kinematic region around $x=10^{-4}$ at larger values of $Q^{2}$.

The l.h.s. of Fig. 1.27 shows the $x$ and $Q^{2}$ coverage for one of the simulated data sets for the spin asymmetry $A_{1}$. The statistical uncertainties are in general way too small to be visible. For the smallest $x$ and $Q^{2}$ values, the expected size of the asymmetries is of the order of a few times $10^{-3}$, which sets the scale for the required experimental precision. On the r.h.s. of Fig. 1.27 we show the $Q^{2}$ dependence of the structure function $g_{1}$ for various bins in $x$. As can be seen, combining the data sets for the different c.m.s. energies extends the coverage in $x$ and $Q^{2}$. We note that present fixed-target data, cf. Fig. 1.25, all fall in the lower right corner of the plot but have some overlap with the projected EIC data.

The pseudo-data for the spin asymmetry $A_{1}$ have been added to a global QCD fit of helicity-dependent PDFs based on the DSSV framework [25, [26]. We have used the projected uncertainties to randomize the pseudo-data by one sigma around their central


Figure 1.27. left: generated pseudo-data for $A_{1}$ in bins of $Q^{2}$ for $5 \times 250 \mathrm{GeV}$ collisions; right: $g_{1}$ as a function of $Q^{2}$ for fixed $x$ for 5 GeV electrons on three different proton energies.


Figure 1.28. $\chi^{2}$ profiles for the truncated $x$ integral of $\Delta g$ (l.h.s.) and uncertainty bands for $x \Delta g$ referring to $\Delta \chi^{2} / \chi^{2}=2 \%$ (r.h.s.) with and without including the generated EIC pseudo-data in the fit.
values determined by the DSSV set of PDFs. To demonstrate the impact of the generated EIC data on $\Delta g$, we show on the l.h.s. of Fig. 1.28 the $\chi^{2}$ profile for the first moment of $\Delta g$ truncated to the range $10^{-4} \leq x<1$ where EIC DIS data with $Q^{2}>1 \mathrm{GeV}^{2}$ can potentially constrain its value. As can be inferred from the plot, the fit based on all presently available DIS, SIDIS, and RHIC $p p$ data set (labeled as "DSSV+" and described in the previous Section) only very marginally constrains the integral. Adding in the projected data for
$5 \times 250 \mathrm{GeV}$, shown in Fig. 1.27, already greatly improves the $\chi^{2}$ profile. Including all four EIC data sets determines the integral very well; recall that the width of the profile determines the uncertainty for a given, tolerated increase $\Delta \chi^{2}$. To achieve such a level of accuracy, the data sets with the highest $\sqrt{s} \simeq 70 \div 80 \mathrm{GeV}$ are most critical in the fit as they probe the smallest $x$ values.

Even more impressive is the reduction of the ambiguities on the $x$ shape of $\Delta g\left(x, Q^{2}\right)$ shown on the r.h.s. of Fig. [1.28, The currently completely undetermined shape for $x \lesssim 0.01$ can be mapped precisely to an accuracy of about $\pm 10 \%$ (or better) for $\gtrsim 10^{-4}$. Below $\approx$ $2 \times 10^{-4}$ the shown $\Delta g\left(x, Q^{2}\right)$ and its uncertainties are not constrained by the projected EIC data and merely result from an extrapolation of the used functional form. We note that since one needs to control all sources of uncertainties extremely well it might be advantageous to measure and analyze polarized cross sections instead of spin asymmetries traditionally used so far. This should greatly simplify the theoretical analysis as one does not need any information on unpolarized PDFs or the ratio of $\sigma_{L} / \sigma_{T}$ anymore. There are also first, very interesting attempts to analyze polarized DIS data within the methodology of neural networks [138, 139], which provides a less biased way to estimate PDF uncertainties than standard approaches based on pre-defined functional forms.

As was mentioned above, one expects to find deviations from DGLAP evolution at sufficiently small values of $x$. In contrast to the unpolarized case, the dominant contribution of gluons mixes with quarks also at $x \ll 1$. From DGLAP evolution one expects for the small $x$ behavior of gluons and quarks

$$
\begin{equation*}
\Delta q\left(x, Q^{2}\right), \Delta g\left(x, Q^{2}\right) \simeq \exp \left[\text { const } \times \alpha_{s} \ln \left(Q^{2} / \mu^{2}\right) \ln (1 / x)\right]^{1 / 2} \tag{1.9}
\end{equation*}
$$

assuming for simplicity a fixed coupling $\alpha_{s}$. In [156, 157] it was demonstrated that this simple behavior can strongly underestimate the rise at small $x$ due to other potentially large double logarithmic contributions of the type $\alpha_{s} \ln ^{2}(1 / x)^{n}$ in the $n$-th order of $\alpha_{s}$ which are beyond the standard DGLAP framework. This gives rise to a power-like behavior of $g_{1}$ at small $x$ of the form $g_{1}\left(x, Q^{2}\right) \sim(1 / x)^{\mathcal{O}\left(\alpha_{s}\right)}$. There are qualitative arguments that in the polarized case the relevance of these logarithms in $1 / x$ is larger than the difference between DGLAP and BFKL evolution in the unpolarized case [156, 157]. However, more detailed quantitative studies are still lacking, and it remains to be seen if the kinematic reach of an EIC is large enough to actually observe deviations from DGLAP in polarized DIS. Clearly, any such estimate will strongly depend upon the initial input distributions, and eventually one needs data to clarify the relevance of small $x$ enhancements. Finally, we note that in Ref. [158] the leading small $x$ logarithms were combined with DGLAP evolution, and some effects of running coupling were addressed in [159].

### 1.11.2 Charm Contribution to $\mathrm{g}_{1}$

As discussed in Sec. 1.7 in the context of unpolarized DIS structure functions, the contributions from heavy flavors require a special theoretical framework. For the kinematic regime covered at the EIC it is expected that effects of the finite heavy quark mass play an important role and should not be neglected. This is, of course, particularly relevant not too far from threshold, i.e., for $Q^{2}$ less than a few times $m_{h}^{2}$.

For all presently available DIS data, the charm contribution to $g_{1}$ can be safely neglected and, hence, is usually not included in any of the QCD analyses except for the fit presented in Ref. [23]. The relevant coefficient functions for $\gamma^{*} g \rightarrow c \bar{c} X$ have been calculated only to LO accuracy [152] so far which is not sufficient for the anticipated experimental precision.


Figure 1.29. LO expectations for $g_{1}^{c}$ (l.h.s.) and $A_{1}^{c}$ (r.h.s) for the $Q^{2}=10 \mathrm{GeV}^{2}, m_{c}=1.35 \mathrm{GeV}$, and using the DSSV and GRSV "std" sets of PDFs. The shaded band corresponds to the $\Delta \chi^{2} / \chi^{2}=2 \%$ uncertainty estimate of DSSV.

The computation of the NLO corrections is, however, work in progress and results should become available for more detailed quantitative studies soon.

For spin dependent DIS the heavy quark contributions are expected to be smaller than in the helicity-averaged case but, of course, will very much depend on the currently unknown size of $\Delta g\left(x, Q^{2}\right)$ at small $x$. There is also an interesting constraint on the gluonic Wilson coefficient for heavy quark production, demanding a vanishing first moment when regulated dimensionally or with a quark mass [160, 161]. This leads to a non-trivial oscillating pattern for $g_{1}^{c}$ depending on the sign of $\Delta g$ which will look rather different in the case that $\Delta g$ itself changes sign within the $x$ range probed.

Figure 1.29 shows some expectations for the spin asymmetry $A_{1}^{c}$ for DIS charm production (r.h.s.) and the charm contribution to the structure function $g_{1}$ (l.h.s.) both computed at LO accuracy with two different polarized gluon distributions. For a small $\Delta g$ with a node, as in the best fit of DSSV, the charm contribution turns out to be at most at the percent level even at collider kinematics, and the corresponding spin asymmetry is most likely too small, $\mathcal{O}\left(\right.$ few $\left.\times 10^{-5}\right)$, to be measured directly. For a larger gluon distribution at small $x$, as in the GRSV fit, or for a gluon within the current uncertainty band of DSSV, asymmetries can be significantly larger, reaching $\mathcal{O}$ (few $\times 10^{-3}$ ), and at $x=10^{-3}$ and $Q^{2} \simeq 10 \mathrm{GeV}^{2}$ charm quarks can contribute about $10 \div 15 \%$ to the inclusive $g_{1}$. The experimental aspects for detecting charmed mesons have beed discussed already in Sec. 1.8 and apply also here.

### 1.11.3 Remark on the Bjorken sum rule

The Bjorken sum rule

$$
\begin{equation*}
\int_{0}^{1} d x\left[g_{1}^{p}\left(x, Q^{2}\right)-g_{1}^{n}\left(x, Q^{2}\right)\right]=\frac{1}{6} C_{B j}\left[\alpha_{s}\left(Q^{2}\right)\right] g_{A} \tag{1.10}
\end{equation*}
$$

is not only one of the most fundamental relations in QCD but presumably also one of the best known quantities in pQCD. Corrections up to $\mathcal{O}\left(\alpha_{s}^{4}\right)$ have been calculated [162, 31, 32]. Given the anticipated precision of DIS measurements at the EIC, it is natural to ask what can be achieved concerning the Bjorken sum. The major obstacle is, of course, the need for an effective, longitudinally polarized neutron beam. One conceivable option would be to run
with ${ }^{3} \mathrm{He}$ but developing a method to measure its polarization to the required percent level is certainly an extremely challenging $R \& D$ task requiring novel ideas. From the theoretical side it might be advantageous to analyze the data not in terms of PDFs but directly on the structure function level with the help of so called "physical anomalous dimensions" 163 . This reduces not only the number of parameters but also theoretical scale uncertainties.


Figure 1.30. The truncated ("running") $x$ integral for the non-singlet combination $\Delta q_{3}$ related to the Bjorken sum normalized to the full first moment for two values of $Q^{2}$.

From present fixed target experiments the sum rule is currently verified to about $10 \%$, which sets the target for any future measurement to the $1 \div 2$ percent level. One of the current limitations is the extrapolation uncertainty from the unmeasured small $x$ region. Since the Bjorken sum probes a non-singlet (NS) quark combination, the small $x$ uncertainties are considerably less severe than for $\Delta g\left(x, Q^{2}\right)$, but to reduce them to a level of about $2 \%$, measurements of $g_{1}^{p, n}$ down to $x \simeq 10^{-4}$ are required. This is illustrated in Fig. [1.30 where we show the "running" $x$ integral for the relevant NS quark combination $\Delta q_{3}$ normalized to its full first moment, assuming the functional form from the DSSV analysis. At the required $1 \div 2 \%$ level of accuracy one might start to see deviations from (1.10) due to isospin and charge symmetry violations. Very little is known about these effects, and, if experimentally feasible, measurements could reveal genuine new insights into the hadronic structure.

The fundamental relation (1.10) between a high-energy measurement of DIS structure functions and a low-energy quantity like the axial charge $g_{A}$ by itself warrants an experimental exploration at the EIC. From a more theoretical perspective one might argue that since $\mathcal{O}\left(\alpha_{s}^{4}\right)$ corrections are available, a precision measurement of the Bjorken sum can be turned into one of the most accurate determinations of $\alpha_{s}$. One can easily convince oneself, however, that this does not work out. Changing $\alpha_{s}$ by about one percent, translates only in a $0.1 \%$ change of the Bjorken sum, which is impossible to resolve experimentally. Perhaps more interesting is the non-trivial connection of the Bjorken sum rule to the Adler $D\left(Q^{2}\right)$ function which naturally appears, for instance, in the $e^{+} e^{-}$annihilation into hadrons [164]. These two, seemingly unrelated quantities are connected through the generalized Crewther relation [145, 32]. For large enough $Q^{2}$, the Adler function can be expanded as a power series in $\alpha_{s}$ like $C_{B j}\left[\alpha_{s}\left(Q^{2}\right)\right]$ in (1.10), and results are available up to $\mathcal{O}\left(\alpha_{s}^{4}\right)$ as well [165].


Figure 1.31. Projected spin asymmetries for pion and kaon production in SIDIS for beam energies of $5 \times 250 \mathrm{GeV}$ and various bins in $Q^{2}$.

The Crewther relation then states for the NS part of the $D$ function that

$$
\begin{equation*}
D\left[\alpha_{s}\left(Q^{2}\right)\right] C_{B j}\left[\alpha_{s}\left(Q^{2}\right)\right]=3\left[1+\frac{\pi \beta\left(\alpha_{s}\right)}{\alpha_{s}} K\left[\alpha_{s}\left(Q^{2}\right)\right]\right] \tag{1.11}
\end{equation*}
$$

where $\beta$ denotes the QCD beta function, and the first four terms in the expansion of $K\left[\alpha_{s}\left(Q^{2}\right)\right]$ are known. The term proportional to $\beta$ in (1.11) describes the deviation from the limit of exact conformal invariance of QCD [145, 166]. We also note that since the Bjorken sum rule can be measured down to small values of $Q^{2}$ it provides a way to define an effective strong coupling constant [167, 168] which is by construction gauge and scheme invariant and approaches the standard running of $\alpha_{s}$ in the perturbative domain.

### 1.11.4 Opportunities in semi-inclusive DIS

As has been mentioned in Sec. 1.10, the flavor separation of polarized PDFs in current fits is largely based on pion and kaon yields in SIDIS. An EIC can easily extend the existing kinematic coverage in the same way as for inclusive DIS. Prerequisites for exploiting SIDIS as a precision tool at the EIC, such as good particle identification and well constrained fragmentation functions, have been already discussed in Sec. 1.5 for the unpolarized case.

Figure 1.31 shows projected data for the longitudinal spin asymmetry in SIDIS with identified pions and kaons in the same $Q^{2}$ bins as used for inclusive DIS studies in Fig. 1.27, The simulation is based on the PEPSI Monte Carlo [155] using the GRSV "std" set of polarised PDFs [24]. The following cuts have been applied to model some detector and acceptance effects: $Q^{2}>1 \mathrm{GeV}^{2}, 0.1<y<0.95$, photon depolarization factor $D(y)>0.1$, $W^{2}>10 \mathrm{GeV}^{2}, 0.2<z<0.8, p_{H}>1.5 \mathrm{GeV}$, and $1^{\circ}<\theta_{H}<179^{\circ}$. The momentum cut on the detected hadron $H$ is placed to ensure to be above the PID Cherenkov threshold. The statistical precision reflects one month of running at the luminosities anticipated for
the first stage of eRHIC. Again, these measurements will be limited by systematic uncertainties, which have to be addressed in detail. In addition to the sources of systematic uncertainties present for inclusive DIS, the detector performance for the identification of different produced hadron species is most critical for SIDIS. Additional sets of data have been generated for other combinations of electron and proton beam energies. They are currently being implemented into the same global QCD analysis framework used to analyze the projected inclusive DIS data above. Plots similar to those for the $\chi^{2}$ profile of the truncated $x$ integral and the $x$ dependent uncertainty bands for $\Delta g\left(x, Q^{2}\right)$ in Fig. 1.28 will be prepared to quantify the impact of SIDIS data on our knowledge of helicity-dependent quark densities. We expect that all light quark and anti-quark flavors, i.e., $\Delta u, \Delta \bar{u}, \Delta d$, $\Delta \bar{d}, \Delta s$, and $\Delta \bar{s}$, can be determined with a precision close to the one obtained for $\Delta g\left(x, Q^{2}\right)$ in Fig. 1.28 ,

Although knowledge of individual quark and anti-quark flavors is in principle not required for an understanding of the proton spin sum rule, where only the total quark singlet $\Delta \Sigma$ enters, it would provide deeper insight into the question why the observed total quark polarization is considerably smaller than in naive quark models. Here, it is essential to understand in detail how sea quarks are polarized, i.e., whether they have a preference for spinning "against" the direction of the proton spin thereby diluting the total quark polarization. Current QCD fits [25, [26] start to reveal rather complicated patters of polarization at medium-to-large $x$ with possible sign changes but the statistical precision and kinematic reach of the fixed-target data is not sufficient for any definitive conclusions.


Figure 1.32. $x(\Delta \bar{u}-\Delta \bar{d})$ at $Q^{2}=10 \mathrm{GeV}^{2}$ along with the uncertainty bands from DSSV, results from earlier global fits, and predictions from the chiral quark soliton model [169, 170].

To give an example, Fig. 1.32 shows the current significance of a possible asymmetry in the light quark sea, $\Delta \bar{u}(x)-\Delta \bar{d}(x)$. Given the well-established pronounced difference between $\bar{u}$ and $d$ in the spin-averaged case, a precise determination of $\Delta \bar{u}(x)-\Delta d(x)$ is of of particular interest. Different patterns of symmetry breaking in the light anti-quark sea polarizations have been predicted qualitatively by a number of models of nucleon structure. For instance, within the large- $N_{c}$ limit of QCD as incorporated in the chiral quark soliton model [169, [170, [171, 172 ] one expects $|\Delta \bar{u}-\Delta \bar{d}|>|\bar{u}-\bar{d}|$. In addition, charged kaon data should help to clarify issues related to $\mathrm{SU}(3)$ symmetry and the polarized strangeness density $\Delta s\left(x, Q^{2}\right)$ by providing sufficient input to determine its first moment reliably.

### 1.12 Electroweak structure functions at the EIC

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### 1.12.1 Motivation and Introduction

The use of charged leptons to probe the structure of nucleons through electroweak interactions has proven to be an invaluable tool in our exploration of the strong force. Experiments on deep inelastic scattering (DIS) $e p \rightarrow e X$, which dominantly proceeds via the exchange of a virtual photon between the electron and the nucleon, have established the existence of quarks and provided detailed studies of the short range aspects of the strong coupling.

It is well known that neutral current ( NC ) interactions can also be mediated by the $Z$-bosons of the weak interactions, and their interference with the photon. This gives rise to parity violating effects, which offer complementary access to nucleon structure. This has been a theme at parity violating electron scattering experiments, both at fixed target facilities [173, 3] and at HERA [174, 175]. For an unpolarized target, the NC parity violating asymmetry is given by

$$
\begin{equation*}
A_{\mathrm{beam}} \equiv \frac{\sigma_{R}-\sigma_{L}}{\sigma_{R}+\sigma_{L}} \tag{1.12}
\end{equation*}
$$

where $\sigma_{R}\left(\sigma_{L}\right)$ denotes the cross section for right- (left-) handed electrons. For fixed-target experiments, where the virtuality $Q$ of the exchanged boson is typically much smaller than the $Z$-boson mass $M_{Z}$, only $\gamma Z$-interference is relevant, and one obtains

$$
\begin{equation*}
A_{\text {beam }} \sim \frac{G_{F} M_{Z}^{2}}{2 \sqrt{2} \pi \alpha} \frac{Q^{2}}{Q^{2}+M_{Z}^{2}} \underset{Q^{2} \ll M_{Z}^{2}}{\simeq} 10^{-4} Q^{2}\left[\mathrm{GeV}^{2}\right], \tag{1.13}
\end{equation*}
$$

with the Fermi constant $G_{F}$ and the fine structure constant $\alpha$. At modern fixed target facilities, measured asymmetries were typically of the order of $10^{-4}$ or less [173]. At HERA, on the other hand, with its enormous kinematic reach in $Q^{2}$, also contributions by pure $Z$-exchange play a role [174].

Charged current (CC) interactions in DIS lepton scattering measurements have been performed at HERA in $e^{ \pm} p$ collisions [174] and at various neutrino scattering experiments [176]. They are inaccessible at fixed target charged lepton beam facilities where $Q^{2} \ll M_{W}^{2}$.

An EIC provides a number of advantages in the study of structure functions through electroweak interactions over previous and existing facilities. As the asymmetries and relative likelihood of $Z^{0}$ and $W^{ \pm}$exchange monotonically increase with $Q^{2}$, larger c.m.s. energies are more favorable for such measurements. Additionally, advances in accelerator and source technologies should provide luminosities on the order of $\sim 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$, two orders of magnitude higher than what was available at HERA. A new feature will be the ability for bunch-by-bunch variation of the sign of the longitudinal polarization of both the electron and hadron beams. A broader $Q^{2}$ and $y$ acceptance than at fixed target facilities, and variable beam energy, also allow for separation of the various structure functions. High precision is possible over a broad range in Bjorken- $x, 0.01 \lesssim x \lesssim 0.4$, whereas fixed target facilities typically are sensitive only to $x>0.1$.

## Polarized Hadrons

Arguably the most important feature at the EIC is the availability of polarized ${ }^{1} \mathrm{H}$, and potentially ${ }^{2} \mathrm{H}$ and ${ }^{3} \mathrm{He}$, beams with rapid polarization flips, which offers access to
electroweak spin structure functions that may provide additional constraints on polarized PDFs. The counterpart of $A_{\text {beam }}$ in (1.12) with polarized protons has never been measured before, and neither have spin asymmetries in CC interactions. Both would in principle be accessible at the EIC.

The theoretical study of electroweak spin-dependent structure functions dates back to the seventies [177, 178, 179, 180, 181, 182, 183, 184, 185]. Renewed interest arose in the nineties in the context of a possible polarized ep program at HERA [186, 187, 188, 189 , 190, 191, 192, 193, 194, 195, 196, 197, 198, and later in terms of studies for a neutrino factory [199. Parity-violating spin structure functions were shown to contain rich information on polarized PDFs. For example, as we shall discuss in more detail in the next section, for CC interactions via $W^{-}$exchange in the parton model, two structure functions $g_{1}^{W^{-}}$and $g_{5}^{W^{-}}$contribute to the spin asymmetry [196, 197]:

$$
\begin{equation*}
A^{W^{-}}=\frac{2 b g_{1}^{W^{-}}+a g_{5}^{W^{-}}}{a F_{1}^{W^{-}}+b F_{3}^{W^{-}}} \tag{1.14}
\end{equation*}
$$

where $a=2\left(y^{2}-2 y+2\right), b=y(2-y)$, and

$$
\begin{equation*}
g_{1}^{W^{-}}(x)=\Delta u(x)+\Delta \bar{d}(x)+\Delta c+\Delta \bar{s}(x), \quad g_{5}^{W^{-}}(x)=-\Delta u(x)+\Delta \bar{d}(x)-\Delta c+\Delta \bar{s}(x) . \tag{1.15}
\end{equation*}
$$

In Eq. (1.14), $F_{1}^{W^{-}}$and $F_{3}^{W^{-}}$are the corresponding unpolarized CC structure functions. Extraction of $g_{1}^{W^{-}}$and $g_{5}^{W^{-}}$hence offers new and independent constraints on the quark and anti-quark helicity distributions, with $g_{1}^{W^{-}}$measuring singlet contributions, while $g_{5}^{W^{-}}$is a flavor non-singlet. If additionally positrons and polarized neutrons are available, which is possible at the EIC, one could obtain a full flavor decomposition of the nucleon polarized quark and anti-quark sector. For instance, for proton scattering $g_{1}^{W^{-}}+g_{1}^{W^{+}}$provides the full quark singlet distribution $\Delta \Sigma$, whose first moment gives the quark and anti-quark spin contribution to the proton's spin. Likewise, $g_{5}^{W^{-}}+g_{5}^{W^{+}}$determines the "valence" distributions $\Delta q-\Delta \bar{q}$. Adding neutrons, one has, for example, $g_{5, p}^{W^{+}, p}-g_{5, n}^{W^{+}, n}=\Delta u+$ $\Delta \bar{u}-(\Delta d+\Delta \bar{d})$, which satisfies a sum rule equally fundamental as the Bjorken sum rule:

$$
\begin{equation*}
\int_{0}^{1} d x\left[g_{5}^{W^{+}, p}-g_{5}^{W^{+}, n}\right]=\left(1-\frac{2 \alpha_{s}}{3 \pi}\right) g_{A} \tag{1.16}
\end{equation*}
$$

where we have included the first-order QCD correction [193]. NC structure functions offer independent insights into nucleon structure. For example, for the $\gamma-Z$ interference contribution, the structure function $g_{1}$ becomes to good approximation $g_{1}^{\gamma Z} \propto \Delta u+\Delta \bar{u}+\Delta d+$ $\Delta \bar{d}+\Delta s+\Delta \bar{s}$ and thus again probes the full quark and anti-quark singlet. The structure function $g_{5}$, on the other hand, probes the valence densities: $g_{5}^{\gamma Z} \propto 2 \Delta u_{v}+\Delta d_{v}$.

We present a few first studies of the prospects for measurements of electroweak spin structure functions in CC and NC scattering at an EIC. These are not meant to present an exhaustive assessment of all the opportunities the EIC would provide in this area.

### 1.12.2 Electroweak Deep Inelastic Scattering

## Structure Functions and Parton Model Expressions

In the determination of cross sections and asymmetries, we follow closely the PDG review 3]. The spin-averaged DIS cross section for $Q^{2} \gg M^{2}$, where $M$ is the mass of the nucleon, is
given by

$$
\begin{equation*}
\frac{d^{2} \sigma^{i}}{d x d y}=\frac{2 \pi \alpha^{2}}{x y Q^{2}} \eta^{i}\left[Y_{+} F_{2}^{i} \mp Y_{-} x F_{3}^{i}-y^{2} F_{L}^{i}\right] \tag{1.17}
\end{equation*}
$$

where $i$ is for NC or CC and $Y_{ \pm}=1 \pm(1-y)^{2}$. We have introduced the longitudinal structure function $F_{L}^{i}=F_{2}^{i}-2 x F_{1}^{i}$, which vanishes to lowest order according to the CallanGross relation. The NC structure functions for $e^{ \pm} N$ scattering can be represented as the sums of the photon, $Z^{0}$, and interference contributions:

$$
\begin{equation*}
F_{2}^{\mathrm{NC}}=F_{2}^{\gamma}-\left(g_{V}^{e} \pm \lambda g_{A}^{e}\right) \eta_{\gamma Z} F_{2}^{\gamma Z}+\left(g_{V}^{e}{ }^{2}+g_{A}^{e}{ }^{2} \pm 2 \lambda g_{V}^{e} g_{A}^{e}\right) \eta_{Z} F_{2}^{Z} \tag{1.18}
\end{equation*}
$$

and

$$
\begin{equation*}
x F_{3}^{\mathrm{NC}}=-\left(g_{A}^{e} \pm \lambda g_{V}^{e}\right) \eta_{\gamma Z} x F_{3}^{\gamma Z}+\left[2 g_{V}^{e} g_{A}^{e} \pm \lambda\left(g_{V}^{e}{ }^{2}+g_{A}^{e} 2\right)\right] \eta_{Z} x F_{3}^{Z} . \tag{1.19}
\end{equation*}
$$

Here and above, the sign $\pm$ is commensurate to the lepton charge. We have

$$
\begin{equation*}
\eta_{\gamma}=1 ; \quad \eta_{\gamma Z}=\left(\frac{G_{F} M_{Z}^{2}}{2 \sqrt{2} \pi \alpha}\right)\left(\frac{Q^{2}}{Q^{2}+M_{Z}^{2}}\right) ; \quad \eta_{Z}=\eta_{\gamma Z}^{2} \tag{1.20}
\end{equation*}
$$

and $g_{V}^{e}=-\frac{1}{2}+2 \sin ^{2} \theta_{W}, g_{A}^{e}=-\frac{1}{2} . \lambda= \pm 1$ is the electron/positron helicity.
The spin-averaged structure functions can be written as

$$
\begin{align*}
& {\left[F_{2}^{\gamma}, F_{2}^{\gamma Z}, F_{2}^{Z}\right]=x \sum_{q}\left[e_{q}^{2}, 2 e_{q} g_{V}^{q}, g_{V}^{q} 2+g_{A}^{q} 2\right](q+\bar{q}),} \\
& {\left[F_{3}^{\gamma}, F_{3}^{\gamma Z}, F_{3}^{Z}\right]=\sum_{q}\left[0,2 e_{q} g_{A}^{q}, 2 g_{V}^{q} g_{A}^{q}\right](q-\bar{q}),} \tag{1.21}
\end{align*}
$$

where $e_{q}$ is the fractional electric charge of the quark, $g_{V}^{q}= \pm \frac{1}{2}-2 e_{q} \sin ^{2} \theta_{W}$, and $g_{A}^{q}= \pm \frac{1}{2}$, with the + sign for up-type quarks and the - sign for down-type quarks.

For $Q^{2} \ll M_{Z}^{2}$, the pure $Z$ contribution can be neglected, and one finds in this limit

$$
\begin{equation*}
A_{\text {beam }}=\frac{G_{F} Q^{2}}{2 \sqrt{2} \pi \alpha}\left[g_{A}^{e} \frac{F_{1}^{\gamma Z}}{F_{1}^{\gamma}}+g_{V}^{e} \frac{Y_{-}}{2 Y_{+}} \frac{F_{3}^{\gamma Z}}{F_{1}^{\gamma}}\right] \tag{1.22}
\end{equation*}
$$

For the case of a polarized target, there are similar spin dependent structure functions. The difference $\Delta \sigma$ of cross sections for the two nucleon helicity states is

$$
\begin{equation*}
\frac{d^{2} \Delta \sigma^{i}}{d x d y}=\frac{8 \pi \alpha^{2}}{x y Q^{2}} \eta^{i}\left[Y_{+} x g_{5}^{i} \pm Y_{-} x g_{1}^{i}-y^{2} g_{L}^{i}\right], \tag{1.23}
\end{equation*}
$$

where again $i$ is for NC or CC and where $g_{L}^{i}=g_{4}^{i}-2 x g_{5}^{i}$. We note that, like $F_{L}$, the latter quantity vanishes to $\mathcal{O}\left(\alpha_{s}^{0}\right)$ [178]. The NC spin dependent structure functions are

$$
\begin{align*}
g_{5}^{\mathrm{NC}} & =-\left(g_{V}^{e} \pm \lambda g_{A}^{e}\right) \eta_{\gamma Z} g_{5}^{\gamma Z}+\left(g_{V}^{e}{ }^{2}+g_{A}^{e}{ }^{2} \pm 2 \lambda g_{V}^{e} g_{A}^{e}\right) \eta_{Z} g_{5}^{Z} \\
g_{1}^{\mathrm{NC}} & =\lambda g_{1}^{\gamma}-\left(g_{A}^{e} \pm \lambda g_{V}^{e}\right) \eta_{\gamma Z} g_{1}^{\gamma Z}+\left(2 g_{V}^{e} g_{A}^{e} \pm \lambda\left(g_{V}^{e}{ }^{2}+g_{A}^{e} 2\right)\right) \eta_{Z} g_{1}^{Z} \tag{1.24}
\end{align*}
$$

Their components can be written as

$$
\begin{align*}
& {\left[g_{1}^{\gamma}, g_{1}^{\gamma Z}, g_{1}^{Z}\right]=\frac{1}{2} \sum_{q}\left[e_{q}^{2}, 2 e_{q} g_{V}^{q}, g_{V}^{q}{ }^{2}+g_{A}^{q}{ }^{2}\right](\Delta q+\Delta \bar{q}),} \\
& {\left[g_{5}^{\gamma}, g_{5}^{\gamma Z}, g_{5}^{Z}\right]=\sum_{q}\left[0, e_{q} g_{A}^{q}, g_{V}^{q} g_{A}^{q}\right](\Delta q-\Delta \bar{q}) .} \tag{1.25}
\end{align*}
$$

The spin asymmetry for scattering an unpolarized lepton off a polarized nucleon is then given by

$$
\begin{equation*}
A_{\mathrm{L}}=\eta^{\gamma Z}\left[g_{V}^{e} \frac{g_{5}^{\gamma Z}}{F_{1}^{\gamma}} \mp \frac{Y_{-}}{Y_{+}} g_{A}^{e} \frac{g_{1}^{\gamma Z}}{F_{1}^{\gamma}}\right] \tag{1.26}
\end{equation*}
$$

In the CC case, we have

$$
\begin{equation*}
\eta_{\mathrm{CC}}=(1 \pm \lambda)^{2} \eta_{W}=\frac{(1 \pm \lambda)^{2}}{2}\left(\frac{G_{F} M_{W}}{4 \pi \alpha} \frac{Q^{2}}{Q^{2}+M_{W}^{2}}\right)^{2} \tag{1.27}
\end{equation*}
$$

For $W^{-}$exchange (electron scattering), the structure functions (assuming four active flavors) are in the parton model:

$$
\begin{align*}
F_{2}^{W-}=2 x(u+\bar{d}+\bar{s}+c), & F_{3}^{W-}=2(u+\bar{d}+\bar{s}+c), \\
g_{1}^{W-}=\Delta u+\Delta \bar{d}+\Delta \bar{s}+\Delta c, & g_{5}^{W-}=-\Delta u+\Delta \bar{d}+\Delta \bar{s}-\Delta c . \tag{1.28}
\end{align*}
$$

For $W^{+}$exchange, one replaces $u \leftrightarrow d$ and $s \leftrightarrow c$. The spin asymmetries for electron and positron scattering then take the simple parton model forms

$$
\begin{equation*}
A_{W^{-}}=\frac{\Delta u+\Delta c-(1-y)^{2}(\Delta \bar{d}+\Delta \bar{s})}{u+c+(1-y)^{2}(\bar{d}+\bar{s})}, \quad A_{W^{+}}=\frac{(1-y)^{2}(\Delta d+\Delta s)-\Delta \bar{u}-\Delta \bar{c}}{(1-y)^{2}(d+s)+\bar{u}+\bar{c}} . \tag{1.29}
\end{equation*}
$$

By measuring over a range in $y$, one can perform a separation of the $\Delta u+\Delta c, \Delta d+\Delta s$ quark or anti-quark combinations.

## Next-to-leading Order QCD Corrections

The NLO QCD corrections to the spin-dependent structure functions have been computed in Refs. [192, 193. To NLO, the expression for a given structure function can be cast into the generic form [199]

$$
\begin{align*}
& g_{1}^{\mathrm{NLO}}\left(x, Q^{2}\right)=\Delta C_{q, 1} \otimes g_{1}^{\mathrm{LO}}+f_{\Sigma} \Delta C_{g} \otimes \Delta g \\
& \frac{g_{4}^{\mathrm{NLO}}\left(x, Q^{2}\right)}{2 x}=\Delta C_{q, 4} \otimes\left[\frac{g_{4}^{\mathrm{LO}}}{2 x}\right], \\
& g_{5}^{\mathrm{NLO}}\left(x, Q^{2}\right)=\Delta C_{q, 5} \otimes g_{5}^{\mathrm{LO}} \tag{1.30}
\end{align*}
$$

where the symbol $\otimes$ denotes a convolution, and $g_{i}^{\mathrm{LO}}$ is the LO (parton model) expression for the respective structure function. The coefficient functions to NLO in the MS scheme can be found in [192, 193]. The factor $f_{\Sigma}$ in Eq. (1.30) is the sum over the coefficient of each quark or anti-quark distribution in the LO expression for $g_{1}$. For example, for the electromagnetic $g_{1}^{\gamma}$ with four flavors, $f_{\Sigma}=10 / 9$, while for $g_{1}^{W^{-}}$one has $f_{\Sigma}=4$. Needless to say that when including the NLO corrections in the calculation of the structure functions, one also has to perform the evolution of the polarized PDFs to NLO [12, 200, 13]. For the most part of our study, we will only use the LO expressions for the structure functions, which are expected to be entirely sufficient for estimating the sensitivities at an EIC. We will, however, briefly investigate the typical size of the NLO corrections in Figs. 1.36 and 1.40 below.


Figure 1.33. Total NC and CC cross sections for $Q^{2}>1 \mathrm{GeV}^{2}$ as functions of the $e p \sqrt{s}$.

### 1.12.3 Measurements of Parton Distribution Functions

In the following, we will present estimates for rates and spin asymmetries for electroweak DIS at an EIC. For the spin-averaged case, we use the CTEQ6.5 [201] unpolarized PDFs. For the helicity PDFs we use the ones of [25]. We note that the latter do not contain a charm quark distribution.

## Basic kinematics and machine considerations

Proposed EIC parameters allow for electron energies of $5-30 \mathrm{GeV}$ and ion energies of $50-325 \mathrm{GeV}$. Figure 1.33 shows the spin-averaged NC and CC total cross sections for electron and positron scattering, as functions of the $e p$ c.m.s. energy $\sqrt{s}$. We have integrated over all $Q^{2}>1 \mathrm{GeV}^{2}$, based on a simple theoretical LO calculation. One can see that the cross section of course rises with energy, but relatively mildly so. Therefore, measurements of electroweak structure functions may well be feasible in collisions at energies significantly lower than those at HERA.

The upper two plots in Figure 1.34 show distributions of the CC cross section in $\log \left(Q^{2}\right)$ and $\log (x)$, respectively, at three different c.m.s. energies. One can see that the largest statistical weight would be at $x \sim 0.1$ and $Q^{2} \sim 1000 \mathrm{GeV}^{2}$, which is a consequence of the $W$-propagator factor in Eq. (1.27). Binning in $x$ and $Q^{2}$ of course allows to investigate more detailed distributions, see below. For NC interactions, the $\gamma$-exchange contribution dominates the spin-averaged cross section and strongly pushes the $Q^{2}$ distribution towards $Q^{2} \rightarrow 0$ (see center row of the figure). Taking the parity-violating electron beam-helicity difference of cross sections, however, essentially singles out the $\gamma Z$-interference contribution. For this piece, which of course is much smaller than the full spin-averaged cross section, the $Q^{2}$ distribution levels off towards $Q^{2} \rightarrow 0$, as follows from the expressions in Sec. 1.12 .2


Figure 1.34. Top row: Distributions of the CC spin-averaged cross section in $Q^{2}$ (left) and $x$ (right). We have applied the cuts $Q^{2} \geq 1 \mathrm{GeV}^{2}$ and $0.1 \leq y \leq 0.9$. Center row: same for the NC case. Bottom row: Same for the NC parity-violating electron beam-helicity difference of cross sections.


Figure 1.35. Left: Total number of CC events for $20 \times 250 e^{-} p$ scattering for an integrated luminosity of $10 \mathrm{fb}^{-1}$. Right: Binned NC event rate as function of the electron scattering angle, for $20 \times 325$ $e^{-} p$ collisions at $\mathcal{L}=1 \times 10^{33} / \mathrm{s} / \mathrm{cm}^{2}$.
and as shown in the bottom row of Fig. 1.34
In CC electron scattering, $e^{-} p \rightarrow \nu_{e} X$, the neutrino remains undetected. To identify a CC event and to reconstruct $x$ and $Q^{2}$, the final-state hadrons must then be reconstructed instead. The detectors must hence be optimized to detect resulting hadronic jet formation. There will likely be some additional detection and reconstruction efficiency associated with this type of analysis. The discussion of the specific requirements is beyond the scope of this study, and we will assume that this reconstruction is possible. In practice, CC measurements could be performed simultaneously with the NC ones, though at a reduced duty factor if the electron helicity is flipped, as the interaction is purely $V-A$. We also assume that polarized positron beams would be available at an EIC.

For the following analysis, we will consider configurations of $E_{e}[\mathrm{GeV}] \times E_{\mathrm{ion}}[\mathrm{GeV}]$ with $20 \times 325$ and $20 \times 250$. For each of these, a luminosity of about $\sim 1 \times 10^{34} / \mathrm{s} / \mathrm{cm}^{2}$ was considered, with estimates for machine availabilities, detector acceptance and efficiency, and beam polarization. Based on an expected five year run time, we consider a realistic effective integrated luminosity of $100 \mathrm{fb}^{-1}$ for NC processes and $10 \mathrm{fb}^{-1}$ for CC. For the studies below, a Monte Carlo simulation framework was developed to evaluate rates and asymmetries of both the NC and CC processes. No detector responses have yet been included, and a full azimuthal acceptance was assumed. In all analyses we consider a minimum scattered electron energy of 2 GeV within $3^{\circ}<\theta<177^{\circ}$ scattering angle. The smaller integrated luminosity for CC studies is because of a factor of 2 loss due to helicity flips and also because efficiency of hadron jet and kinematic reconstruction has not yet been studied.

Of practical importance is to evaluate how well a separation of the structure functions can be done at individual points in $x$, though it remains for a future Monte Carlo study to evaluate the $x$ resolution after reconstruction. We bin all data in $20 x$ bins logarithmically spaced from $10^{-5}$ to 1 . When binned in $Q^{2}$, we use 20 bins from 2 to $5 \times 10^{4} \mathrm{GeV}^{2}$. These $Q^{2}$ bins were also used in determining any $y$ dependence. Figure 1.35 (left) shows the total number of events expected for CC interactions in $e^{-} p$ scattering at $\sqrt{s}=141 \mathrm{GeV}$ and $\mathcal{L}=10 \mathrm{fb}^{-1}$, binned in $x$.

Typical rates in NC scattering are up to 1 kHz , as shown in the right part of Fig. 1.35 for $\sqrt{s}=161 \mathrm{GeV}$. The highest rate occurs in the forward direction of the electron beam. Here, pipeline electronics will likely be necessary in order to avoid significant deadtime effects.


Figure 1.36. CC spin dependent structure functions $g_{1}^{W^{-}}, g_{5}^{W^{-}}$, and $g_{4}^{W^{-}} / 2 x$, at $Q^{2}=100 \mathrm{GeV}^{2}$. The dashed lines show the LO results (the one for $g_{4}^{W^{-}} / 2 x$ is not shown in this case, since it coincides with that for $g_{5}^{W^{-}}$), while the solid curves are NLO. For comparison, we also show the electromagnetic $g_{1}^{\gamma}$.

## Polarized Parton Distributions from CC Interactions

As follows from Eq. (1.29), CC processes in electron scattering off polarized targets offer a unique method to extract combinations of $\Delta u+\Delta c$ and $\Delta \bar{d}+\Delta \bar{s}$. With positron beams, one could also extract $\Delta d+\Delta s$ and $\Delta \bar{u}+\Delta \bar{c}$. For the present analysis, we have assumed a $100 \%$ polarized electron/positron source. As mentioned before, we have assumed only $10 \mathrm{fb}^{-1}$ integrated luminosity, making our estimates somewhat conservative.

In Fig. 1.36 we show the spin structure functions $g_{1}^{W^{-}}, g_{5}^{W^{-}}$, and $g_{4}^{W^{-}} / 2 x$, at $Q^{2}=$ $100 \mathrm{GeV}^{2}$, using the PDFs of [25]. Results are shown both at LO (dashed) and at NLO (solid). One observes that the NLO corrections are well under control. To guide the eye, also the ordinary electromagnetic structure function $g_{1}^{\gamma}$ is shown. Figure 1.37(left) displays the asymmetry $A_{W^{-}}$for CC $e^{-} \vec{p}$ scattering, as function of $x$. Different data points at same $x$ correspond to different bins in $Q^{2}$. As mentioned above, we have chosen here 20 bins in $Q^{2}$, spaced logarithmically from $2 \mathrm{GeV}^{2}$ to $5000 \mathrm{GeV}^{2}$. The lower asymmetries correspond to the lower bins in $Q^{2}$. Thanks to the simple structure of the LO expressions for the cross sections, the asymmetries in CC interactions become very large in the valence region, much larger than those in the NC case to be discussed below. On the other hand, as we saw in Figs. 1.34 and 1.35, event rates are much more suppressed at lower $Q^{2}$ and therefore $x$. The right part of Fig. 1.37 gives the resulting values for the relative uncertainty $\delta A_{W^{-}} / A_{W^{-}}$ of the asymmetry. Here we have summed over all $Q^{2}$ bins. The results shown look very promising, with better than $10 \%$ measurements appearing feasible all the way down to $x \sim 10^{-2}$. It is worth keeping in mind that relative polarimetry uncertainties at an EIC are also expected to be at the $0.5-1 \%$ level for electrons and $2-3 \%$ level for hadrons, so that these might become the dominant sources of uncertainty in the regions where the statistical $\delta A_{W^{-}} / A_{W^{-}}$is very small, especially at high $x$.

Using Eq. (1.29), the asymmetries give direct access to the polarized quark and antiquark distributions. As we discussed, higher-order QCD corrections (and also Cabibbosuppressed contributions) will somewhat modify the expressions in Eq. (1.29). However, for a first estimate use of Eq. (1.29) as a means to gauge the sensitivity to the distributions


Figure 1.37. Left: spin asymmetry for $\mathrm{CC} e^{-} \vec{p}$ scattering, as function of $x$ for various bins in $Q^{2}$. Right: resulting relative uncertainties of the asymmetry.
is justified. The additional contributions will not make a qualitative difference and can be systematically included in future studies. If furthermore full knowledge of the unpolarized parton distributions is assumed, then extraction of the sums of the two up-type quarks and down-type anti-quarks can be performed by a linear fit in $(1-y)^{2}$. The results of such fits are shown for electron and positron running in Figs. 1.38 and 1.39, respectively. We note that if a polarized deuterium or ${ }^{3} \mathrm{He}$ beam were available, additional opportunities would arise; $e^{-} \vec{n}$ scattering would probe the combinations $\Delta u+\Delta d+2 \Delta c$ and $\Delta \bar{d}+\Delta \bar{u}+2 \Delta \bar{s}$. At larger $x$ where the sea quarks are suppressed relative to the valence quarks, $e^{-} \vec{p}$ and $e^{-} \vec{n}$ scattering could be used to separate the valence polarizations.

## Structure Functions and Polarized PDFs from NC Interactions

Again we first show the spin-dependent structure functions; see Figure 1.40. As the contributions from pure $Z$-exchange are small, we only consider the electromagnetic $g_{1}^{\gamma}$, and the $\gamma-Z$ interference contributions $g_{1}^{\gamma Z}$ and $g_{4,5}^{\gamma Z}$, whose expressions were given in Eq. (1.25).

The left part of Fig. 1.41 shows the parity-violating spin asymmetry in Eq. (1.22), obtained for a polarized lepton beam scattering off an unpolarized proton beam, as function of $x$ in various different $Q^{2}$ bins. The lower (upper) asymmetries correspond to $Q^{2} \sim 2 \mathrm{GeV}^{2}$ $\left(Q^{2} \sim 4000 \mathrm{GeV}^{2}\right)$. As one can see, typical asymmetries range from $10^{-4}$ to 0.1 . The right part of the figure gives the resulting values for the relative uncertainty $\delta A_{\text {beam }} / A_{\text {beam }}$ of the asymmetry. Here we have summed over all $Q^{2}$ bins and assumed an integrated luminosity of $\mathcal{L}=100 \mathrm{fb}^{-1}$. The relative uncertainty is found to be near $2 \%$ over a relatively wide range in $x$; the relative electron polarization uncertainty achievable with modern polarimetry techniques should be better than this.

According to Eq. (1.22), measurement of the asymmetry $A_{\text {beam }}$ gives access to $F_{1}^{\gamma Z}$ and $F_{3}^{\gamma Z}$. Figure 1.42 presents the expected relative uncertainties for these structure functions, corresponding to the results shown in Fig. 1.41. Figure 1.43 shows the corresponding result for the case of $\vec{e}^{-} D$ scattering, for the structure function $F_{1}^{\gamma Z}$. Due to the suppression by the electron vector coupling, the uncertainty of $F_{3}^{\gamma Z}$ is about an order of magnitude worse than that of $F_{1}^{\gamma Z}$. The sensitivity is maximized in the region of $x \sim 0.01-0.4$. The approved PVDIS experiment using the SoLID spectrometer in Hall A at Jefferson Lab [202] anticipates achieving an extraction of $A_{\text {beam }}$ with relative accuracy $\approx 0.5-1 \%$ over several bins in $x$ in the range of $0.2 \leq x \leq 0.7$, both from proton and deuterium targets. The


Figure 1.38. Top: LO extraction of polarized quark and anti-quark distributions from the spin asymmetry for CC $e^{-} \vec{p}$ scattering. Bottom: Corresponding relative uncertainties of the extracted distributions.


Figure 1.39. Same as Fig. 1.38 but for $e^{+} \vec{p}$ scattering.


Figure 1.40. NC spin-dependent structure functions for $\gamma-Z$ interference, at $Q^{2}=100 \mathrm{GeV}^{2}$, calculated at LO (dashed) and NLO (solid), using the polarized PDFs of 25].



Figure 1.41. Left: Parity violating NC spin asymmetries for polarized electrons on unpolarized protons, binned logarithmically in $x$ and $Q^{2}$. Right: Resulting relative uncertainties of the asymmetry.


Figure 1.42. Relative uncertainties of $F_{1}^{\gamma Z}$ (left) and $F_{3}^{\gamma Z}$ (right) extracted from NC $\vec{e}-p$ scattering.


Figure 1.43. Same as left part of Fig. 1.42 , but for $\vec{e}^{-} \mathrm{D}$ scattering.


Figure 1.44. Same as Fig. 1.41, but for unpolarized electrons on polarized protons.
products of the quarks' electric charges and their vector charges are approximately equal for up-type and down-type quarks, $e_{u} g_{V}^{u} \approx e_{d} g_{V}^{d} \approx 0.1$. Therefore, one has from Eq. (1.21) that $F_{1}^{\gamma Z} \propto u+\bar{u}+d+\bar{d}+s+\bar{s}$, both for proton and deuterium. On the other hand, for the corresponding products of the charges and axial charges one finds $e_{u} g_{A}^{u} \approx 2 e_{d} g_{A}^{d}$, and hence in the valence region $F_{3}^{\gamma Z} \propto 2 u_{v}+d_{v}$ for protons and $\propto u_{v}+d_{v}$ for deuterium. While $F_{3}^{\gamma Z}$ could thus give a clean separation of the $u$ and $d$ valence distributions, its contribution to the beam asymmetry is unfortunately suppressed.

Of significant interest are measurements of $g_{1}^{\gamma Z}$ and $g_{5}^{\gamma Z}$, which contain complementary information on the polarized PDFs. Similarly to what we discussed for the case of $F_{1}^{\gamma Z}$, one finds that to a good approximation $g_{1}^{\gamma Z} \propto \Delta u+\Delta \bar{u}+\Delta d+\Delta \bar{d}+\Delta s+\Delta \bar{s}$, which would in principle make this structure function an complementary probe of the quark and anti-quark singlet and spin contribution to the proton spin. Furthermore, $g_{5}^{\gamma Z}$ offers probes of the valence regime. According to Eq. (1.23), $g_{1}^{\gamma^{Z}}$ and $g_{5}^{\gamma Z}$ may be accessed by flipping the proton helicity while leaving the electron polarization unchanged. The corresponding spin asymmetries, obtained after summing over the electron helicities, are unfortunately overall much smaller than their counterparts with polarized electron and unpolarized proton. They are shown in Fig. 1.44, along with the their expected relative uncertainties, computed again for $\mathcal{L}=100 \mathrm{fb}^{-1}$. The best sensitivity is in the valence quark region, $x>0.1$. Even here, it remains at the $10 \%$ level. This directly translates into similar uncertainties for the structure functions $g_{1}^{\gamma Z}$ and $g_{5}^{\gamma Z}$, which are shown in Fig. 1.45. In the valence region, where


Figure 1.45. Structure functions $g_{1}^{\gamma}$ and $g_{5}^{Z Z}$ (top) and their relative uncertainties resulting from Fig. 1.44 (bottom).
sea quarks are irrelevant, we have $g_{1}^{\gamma Z} \propto \Delta u_{v}+\Delta d_{v}$ and $g_{5}^{\gamma Z} \propto 2 \Delta u_{v}+\Delta d_{v}$, which may provide a separation of $\Delta u$ and $\Delta d$.

Finally, assuming perfect knowledge of $\Delta u$ and $\Delta d$ and their anti-quark distributions from other sources, one might ask if an extraction of $\Delta s+\Delta \bar{s}$ from $g_{1}^{\gamma Z}$ and $g_{5}^{\gamma Z}$ could be possible. This quantity, and in particular its integral, is a key ingredient to nucleon spin structure and for understanding why quarks and anti-quarks combined appear to carry little of the proton spin. Constraints on $\Delta s+\Delta \bar{s}$ are presently available from an $\mathrm{SU}(3)$ symmetry analysis of hyperon $\beta$-decays, and from kaon production in semi-inclusive DIS, which are both inflicted with sizable uncertainties and in fact show some tension (for discussion, see [26]). The result for the extraction of $\Delta s+\Delta \bar{s}$ from electroweak DIS at the EIC is shown in Fig. 1.46. As can be seen, a non-zero measurement would be challenging for the assumed $100 \mathrm{fb}^{-1}$ integrated luminosity. Nevertheless, this measurement might become interesting if independent methods of extracting $\Delta s+\Delta \bar{s}$ were to provide surprising results. If this measurement is deemed sufficiently interesting and important, larger integrated luminosities will indeed help, since the measurement will continue to remain statistics limited, provided relative hadron polarization errors can be kept at the $3 \%$ level or better.

### 1.12.4 Summary

We have performed a basic analysis of the potential of an EIC in terms of measurements of structure functions in electroweak NC and CC scattering. Precise measurements of the CC functions $F_{1}^{W}, F_{3}^{W}, g_{1}^{W}$, and $g_{5}^{W}$ become feasible with a relatively modest integrated luminosity. These measurements will greatly aid the flavor decomposition of polarized and


Figure 1.46. Results for the $x(\Delta s+\Delta \bar{s})$ distribution extracted from the $A_{\mathrm{L}}$ spin asymmetry under the assumption that all other helicity distributions are known.
unpolarized PDFs in the region $x \gtrsim 0.01$. NC structure functions become accessible with good precision at high integrated luminosities. Measurements of $F_{1}^{\gamma Z}$ and $F_{3}^{\gamma Z}$ seem to be of limited use in improving present or approved measurements. At the highest luminosities and center of mass energies, $g_{1}^{\gamma Z}$ and $g_{5}^{\gamma Z}$ become accessible; these structure functions have never before been measured. The combined analysis of the new CC and NC structure functions with electrons and positrons as well as with polarized protons and neutrons at these highest luminosities could potentially open a new window into precision QCD tests of the spin structure of the nucleon; this will be the focus of future experimental and theoretical investigations.

### 1.13 Charged current charm production and the strange sea

Marco Stratmann

### 1.13.1 Basic idea

The leading order contribution to CC charm production in $e^{+} p$ DIS is given by the $\mathcal{O}\left(\alpha_{s}^{0}\right)$ parton model process $W^{+} s^{\prime} \rightarrow c$, where $s^{\prime}$ denotes the Cabibbo-Kobayashi-Maskawa (CKM) "rotated" combination $s^{\prime} \equiv\left|V_{c s}\right|^{2} s+\left|V_{c d}\right|^{2} d$. Due to the smallness of $\left|V_{c d}\right|^{2}$ [3] the process is expected to be essentially sensitive to the strange sea content. Only at large $x$, where quark sea contributions are less relevant, the $\left|V_{c d}\right|^{2}$ suppression is balanced by the valence enhancement of the well-known $d(x)$ density. Likewise, in $e^{-} p$ DIS, the process $W^{-} \bar{s}^{\prime} \rightarrow \bar{c}$ predominantly probes the anti-strange density $\bar{s}(x)$. With a polarized proton beam one can access also $\Delta s(x)$ and $\Delta \bar{s}(x)$.

Current determinations of $s(x)$ rely mainly on fixed-target neutrino scattering off nuclear targets with potentially large uncertainties, see Fig. 1.9 in Sec. 1.5. Much less is known about the longitudinally polarized $\Delta s(x)$ so far, see Sec. 1.10. Due to the limited luminosity and charm detection efficiency, charm production in CC DIS could not be studied at HERA. CC DIS would provide an independent way to extract the unpolarized and polarized strange sea distributions at much larger scales, typically $Q \sim M_{W}$, than probed in semi-inclusive kaon production, cf. Sec. 1.5. On the downside, such a measurement requires also a positron beam, though not polarized.

Next-to-leading order QCD corrections also complicate the simple picture for CC charm production and may deteriorate the sensitivity to strangeness. Apart from the $\mathcal{O}\left(\alpha_{s}\right)$ corrections to the LO process $W^{+} s^{\prime} \rightarrow c$, the genuine NLO, gluon induced subprocess $W^{+} g \rightarrow c \bar{s}^{\prime}$ has to be taken into account as well. It contributes significantly to the charm production cross section in certain regions of phase space and hence dilutes the sensitivity to the strange sea. In addition, a proper theoretical calculation also needs to take into account the mass of the produced heavy (charm) quark, as was also discussed in the context of $F_{2, L}^{c}$ in Sec. 1.7 . In order to make contact with experiment, a fully inclusive calculation [203, 111] is not entirely sufficient, and one should compute also the momentum $z$ spectrum of the detected charmed $D$ mesons. In the unpolarized case this was achieved in [204]. The corresponding polarized results can be found in Ref. [205. Imposing a lower cut $z_{\text {min }}$ on the $D$ meson momentum fraction was shown to considerably reduce gluon-initiated NLO contributions and enhance the sensitivity to the strange sea.

Concerning the mass $m_{c}$ of the charm quark, it turns out that the naive "rescaling prescription" [206], i.e., $s(x) \rightarrow s(\xi)$ where $\xi \equiv x\left(1+m_{c}^{2} / Q^{2}\right)$, applies also at NLO accuracy as it allows for a consistent factorization of all initial-state collinear singularities.

### 1.13.2 Sensitivity to the Strange Sea

So far, detailed phenomenological studies have been provided only for HERA kinematics [205], and they still need to be updated for EIC kinematics. However, these projections are sufficient to demonstrate the idea of the measurement and give a rough estimate of the size of cross sections and spin asymmetries. From the studies of inclusive CC electroweak DIS structure functions in Sec. 1.12 we already know that such measurements appear to be feasible at an EIC despite its lower c.m.s. energy than HERA even with moderate integrated luminosities of about $10 \mathrm{fb}^{-1}$.


Figure 1.47. The $z$ integrated polarized cross section for CC charm production in $e^{-} p$ and $e^{+} p$ collisions and the corresponding spin asymmetry $A^{D}$ for ( $\mathbf{a}, \mathbf{b}$ ): $0<z<1$, ( $\mathbf{c}, \mathbf{d}$ ): $0.2<z<1$, using the GRSV "std" and "val" sets of PDFs. Projected uncertainties are for $70 \%$ polarization, $100 \%$ charm detection efficiency, and an integrated luminosity of $5 \mathrm{fb}^{-1}$.

As an example, Fig. 1.47 shows the sensitivity of CC charm ( $D$ meson) production in $e^{-} p$ and $e^{+} p$ collisions at $\sqrt{S}=300 \mathrm{GeV}, Q^{2}>500 \mathrm{GeV}^{2}$, and $0.01 \leq y \leq 0.9$, to the choice of $\Delta s$. The momentum fraction of the detected $D$ meson has been integrated using $z_{\min }=0$ (upper row) and 0.2 (lower row). The GRSV valence set [24] has a very small positive $\Delta s(x)$ in the relevant region $x \gtrsim 0.01$, roughly comparable to what is nowadays obtained from fixed target SIDIS data, e.g., in the DSSV analysis [25, 26]; see Sec. 1.10, On the contrary, the GRSV standard set has a sizable negative strangeness polarization as favored by fits including only inclusive DIS data [23]. Other PDFs, in particular the gluon density, are very similar in both GRSV sets. Note that $\Delta s(x)=\Delta \bar{s}(x)$ is assumed in all current polarized PDF analyses due to the lack of data constraining them separately.

The solid and dashed lines in Fig. 1.47 show the results for $e^{-} p$ scattering for GRSV standard and valence PDFs, respectively. Within the projected statistical uncertainties, obtained for $70 \%$ proton polarization, $100 \%$ charm detection efficiency, and an integrated luminosity of $5 \mathrm{fb}^{-1}$, differences in $\Delta \bar{s}(x)$ can be easily resolved. The dot-dashed and dotted lines show the results for a corresponding measurement with positron beams. Having results for both $W^{-}$and $W^{+}$exchange, one should be able to study a possible asymmetry in $\Delta s(x)-$ $\Delta \bar{s}(x)$. The results presented here need to be backed up with more detailed simulations of CC charm production for EIC kinematics.

### 1.14 Photoproduction processes at an EIC

Hubert Spiesberger, Marco Stratmann

The production of hadronic final states in ep collisions is dominated by photoproduction where the electron is scattered by a small angle producing photons of almost zero virtuality $\left(Q^{2} \simeq 0\right)$. At LO of pQCD , the dominant process for the production of high- $p_{T}$ hadrons, jets, or heavy quarks is often photon-gluon fusion, $\gamma g \rightarrow q \bar{q}$. Here, the photon interacts directly with a gluon from the nucleon. Besides this so-called "direct" photoproduction channel, the scattering can proceed also via "resolved" processes. In this case, the photon acts as a source of partons which interact with the partons in the nucleon through any of the standard $2 \rightarrow 2$ LO QCD hard scattering processes such as $g g \rightarrow g g$ or $q \bar{q} \rightarrow q \bar{q}$. The large number of possible subprocesses can make the resolved contribution sizable in certain regions of phase space. Examples for a direct and a resolved process are shown in Fig. 1.48.

At LO, the two interaction mechanisms in Fig. 1.48 both contribute at $\mathcal{O}\left(\alpha_{e m} \alpha_{s}\right)$ but otherwise appear to be independent. Starting from NLO, however, the separation into direct and resolved contributions becomes factorization scheme dependent. This is due to soft and collinear singularities appearing in a perturbative approach. These singularities have to be identified and consistently factorized into non-perturbative PDFs of the nucleon and the photon. This procedure is not unique, and it is therefore important that the direct and resolved parts are treated together consistently. Only their sum is an experimentally meaningful and measurable cross section. For a theoretical review on photoproduction, see, e.g., Ref. [208].

The differential cross section for electron-nucleon scattering, $d \sigma_{e N}$, at a c.m.s. energy $\sqrt{s}$ is related to the photoproduction cross section $d \sigma_{\gamma N}$ through

$$
\begin{equation*}
d \sigma_{e N}(\sqrt{s})=\int_{y_{\min }}^{y_{\max }} d y f_{e \gamma}(y) d \sigma_{\gamma N}(y \sqrt{s}) . \tag{1.31}
\end{equation*}
$$

Here, $f_{e \gamma}$ is the energy spectrum of the exchanged photon which in the Weizsäcker-Williams approximation is given by

$$
\begin{equation*}
f_{e \gamma}(y)=\frac{\alpha_{e m}}{2 \pi}\left[\frac{1+(1-y)^{2}}{y} \ln \frac{(1-y) Q_{\max }^{2}}{y^{2} m_{e}^{2}}+2(1-y)\left(\frac{y m_{e}^{2}}{(1-y) Q_{\max }^{2}}-\frac{1}{y}\right)\right] . \tag{1.32}
\end{equation*}
$$

The photon flux $f_{e \gamma}$ depends $y=E_{\gamma} / E_{e} . Q_{\max }$ and the range $y_{\min } \leq y \leq y_{\max }$ are determined by cuts in the experimental analysis. Typically, a lower cut $y_{\text {min }}=\mathcal{O}(0.1)$ is


Figure 1.48. Example of a gluon-initiated direct and resolved contributions to photoproduction at LO (taken from Ref. [207]).
applied in order to exclude low-mass hadronic final states, and an upper limit on $y$, e.g., $y_{\max }=0.7 \div 0.9$, is used to reduce the kinematic range where radiative corrections are expected to be large.

The photoproduction cross section is then obtained as the sum of its direct and resolved parts, $d \sigma_{\gamma N}=d \sigma_{\gamma N}^{\mathrm{dir}}+d \sigma_{\gamma N}^{\text {res }}$, as convolutions $\otimes$ of the appropriate partonic hard scattering cross sections $d \sigma_{a b}$ with the PDFs $f_{a / \gamma}\left(x_{\gamma}\right)$ and $f_{b / N}\left(x_{N}\right)$ of the photon and nucleon, respectively, at a factorization scale $\mu_{f}$, i.e.,

$$
\begin{equation*}
d \sigma_{\gamma N}^{\mathrm{res}}=\sum_{a, b} f_{a / \gamma}\left(x_{\gamma}, \mu_{f}\right) \otimes f_{b / N}\left(x_{N}, \mu_{f}\right) \otimes d \sigma_{a b}\left(x_{\gamma}, x_{N}, \mu_{f}\right) . \tag{1.33}
\end{equation*}
$$

$d \sigma_{\gamma N}^{\text {dir }}$ can be obtained from (1.33) by replacing the photon PDFs by a $\delta$-function and considering only photon-parton scattering processes $d \sigma_{\gamma b}$ in the sum.

The resolved process is accompanied by a hadronic remnant of the photon which carries the fraction $1-x_{\gamma}$ of the photon energy. At LO, the presence of a hadronic remnant could be used to distinguish different event topologies for the two mechanisms. In addition, for two-jet final states $x_{\gamma}$ can be reconstructed experimentally from the measured transverse momenta and rapidities of the jets. It is customary to define

$$
\begin{equation*}
x_{\gamma}^{\mathrm{obs}} \equiv\left(E_{\mathrm{T}}^{\mathrm{jet}} e^{-\eta^{\mathrm{jet}} \mathrm{t}_{1}}+E_{\mathrm{T}}^{\mathrm{jet} t_{2}} e^{-\eta^{\mathrm{jet}} \mathrm{t}_{2}}\right) /\left(2 y E_{e}\right) . \tag{1.34}
\end{equation*}
$$

However, at higher orders of pQCD , initial- and final-state radiation of additional partons will also give rise to hadrons emitted in the direction of the incoming photon. Moreover, non-perturbative hadronization may contribute to the appearance of hadrons in the same kinematic region. Both effects lead to a reduction of the experimentally determined value of $x_{\gamma}$. Therefore a unique separation of the direct and resolved parts is not possible anymore. Nevertheless, the variable $x_{\gamma}$ can still be used to define kinematic regimes where direct (large $x_{\gamma}$ ) or resolved (small $x_{\gamma}$ ) contributions dominate.

At HERA, photoproduction has been used to test pQCD and the presence of both direct and resolved photon processes for final-states comprising hadrons, jets, prompt photons, and heavy quarks. Generally, the data are well described by NLO calculations in regimes expected to be dominated by the direct process. Kinematic regions where resolved processes are sizable are somewhat less well described; for a review see, e.g., [209]. This is mainly due to the fact that the photon PDFs needed for the calculation of the resolved contribution are significantly less well constrained by data than the partonic structure of protons. Only data for inclusive DIS off a quasi-real photon target, i.e., $\gamma^{*}\left(Q^{2}\right) \gamma$ scattering in $e^{+} e^{-}$[210], have been used in fits of photon PDFs so far, see, e.g., [211]. No attempts have been made to perform global analyses or to quantify uncertainties at a level similar to current fits of proton PDFs. Any additional, more precise data are therefore of vital importance for an improved understanding of the theoretical description of photoproduction processes and a reliable determination of photon PDFs. The latter are of great phenomenological relevance at a possible future linear $e^{+} e^{-}$collider to describe processes involving quasi-real photons.

The next two sections show some examples how an EIC can contribute to further our knowledge of photoproduction processes both in unpolarized and in polarized electronproton scattering.

### 1.15 Expectations for charm quark photoproduction

Hubert Spiesberger

The description of heavy quark production in the framework of perturbative QCD is complicated due to the presence of several large scales, like the transverse momentum $p_{T}$ of the produced charmed meson, the momentum transfer $Q$ in DIS, or the mass of the produced heavy hadron. Depending on the kinematic range considered, the mass $m_{c}$ of the charm quark may have to be taken into account. Different calculational schemes (see, e.g. [212, [213], and references therein) have been developed to obtain predictions from pQCD, depending on the specific kinematical region and the relative importance of the different scales.

In the case of relatively small transverse momentum, $p_{T} \lesssim m_{c}$, the fixed-flavor number scheme (FFNS) is usually applied. Here one assumes that the light quarks and the gluon are the only active flavors and the charm quark appears only in the final state. The charm quark mass can explicitly be taken into account together with the $p_{T}$ of the produced heavy meson; this approach is therefore expected to be reliable when $p_{T}$ and $m$ are of the same order of magnitude.

In the complementary kinematical region where $p_{T} \gg m_{c}$, calculations are usually based on the zero-mass variable-flavor-number scheme (ZM-VFNS) where $m_{c}=0$ and the charm quark acts as an active parton with its own PDF; see also Sec. 1.7. The charmed meson is produced not only by fragmentation from the charm quark but also from the light quarks and the gluon. The fragmentation process is described with the help of scale-dependent fragmentation functions (FFs), $D(z, \mu)$, which determine the probability that the produced heavy meson carries the fraction $z$ of the momentum of the parton it is produced from. The predictions obtained in this scheme are expected to be reliable only in the region of large $p_{T}$ since all terms of the order $m_{c}^{2} / p_{T}^{2}$ are neglected in the hard scattering cross section.

A unified scheme that combines the virtues of the FFNS and the ZM-VFNS is the so-called general-mass variable-flavour-number scheme (GM-VFNS) [212, 213]. In this approach the large logarithms $\ln \left(p_{T}^{2} / m_{c}^{2}\right)$ are factorized into the PDFs and FFs and summed to all orders by the well-known DGLAP evolution equations. At the same time, massdependent power corrections are retained in the hard-scattering cross sections, as in the FFNS. In order to conform with standard $\overline{\mathrm{MS}}$ factorization, finite subtraction terms must be supplemented to the results of the FFNS. As in the ZM-VFNS, one has to take into account processes with incoming charm quarks, as well as light quarks and gluons in the final state which fragment into the heavy meson. It is expected that this scheme is valid not only in the region $p_{T}^{2} \gg m_{c}^{2}$, but also in the kinematic region where $p_{T}$ is only a few times larger than $m_{c}$. The basic features of the GM-VFNS are described in Ref. [214]. Analytic results for the required hard scattering cross sections can be found in Refs. [213, 215, 216, 217.

Next, we present theoretical predictions [214] for the photoproduction of $D^{*}$-mesons in $e p$ scattering at the EIC. We assume an experimental analysis with $Q_{\max }=1 \mathrm{GeV}$ in Eq. (1.32). Since the cross section is dominated by low $Q^{2}$, our results should not depend too strongly on the precise value of $Q_{\max }$. The relevant direct and resolved hard scattering cross sections are calculated at NLO accuracy. For the photon PDFs we use the parametrization of Ref. [218] with the standard set of parameter values, and for the proton PDF we have chosen the CTEQ6.5 set [201]. For the FFs we use the Global-GM set of Ref. [219] based on a fit to the combined Belle [220], CLEO [221], ALEPH [222], and OPAL [223, 224] data. We choose the renormalization and factorization scales to be equal and use $\mu_{r}=\mu_{f}=m_{T}$,


Figure 1.49. $d \sigma / d \eta$ for the production of $D^{*}$ mesons at the EIC for two settings of beam energies integrated over transverse momenta $3 \mathrm{GeV} \leq p_{T} \leq 5 \mathrm{GeV}$. The different curves are explained in the text.
where $m_{T}=\sqrt{m_{c}^{2}+p_{T}^{2}}$ is the transverse mass and $m_{c}=1.5 \mathrm{GeV}$. In Ref. [214] we studied scale uncertainties for photoproduction at HERA, as well as ambiguities due to various possible choices for input variables, such as the proton and photon PDFs, the $D^{*}$ FFs, and the dependence on $m_{c}$.

In our calculation of the differential cross section $d \sigma / d \eta$ (where $\eta$ is the rapidity of the observed heavy meson, $D^{* \pm}$ ) we use $E_{p}=325 \mathrm{GeV}$ and consider two choices for the energy of the electron beam: $E_{e}=5 \mathrm{GeV}$ (left panel of Fig. 1.49) and $E_{e}=30 \mathrm{GeV}$ (right panel). The transverse momentum $p_{T}$ is integrated over the range $3<p_{T}<5 \mathrm{GeV}$. The results show that the higher electron beam energy would lead to an increase of the cross section by roughly a factor of three and the rapidity distribution is shifted towards the backwards region, as expected.

The figure shows a split-up of the total cross section into contributions from different subprocesses. From top to bottom, the curves correspond to the total cross section (full line), the direct contribution (long dashed), the total resolved part (dotted), the contribution due to charm in the photon (dash-dot-dotted) and charm in the proton (long double-dashed), and, finally, the part due to resolved subprocesses with light partons in the initial state. The direct contribution, which is sensitive mainly to the gluon distribution in the proton, is dominating throughout the shown range of $p_{T}$ and $\eta$. The resolved part is mainly due to the charm content of the photon, in particular, at negative rapidities. Here one may hope that measurements at an EIC, in particular, for the option with the highest $\sqrt{s}$, will contribute to a better determination of the photon PDFs.

The total cross sections for charm production at an EIC are not very different from those measured at HERA; however, an increase in the precision of corresponding measurements can be expected due to the higher luminosity. Apart from providing a better testing-ground for pQCD , one may expect that the experimental information will contribute to an improved determination of the charm content of the proton and, perhaps, the charm FFs.

### 1.16 Polarized photoproduction at an EIC

Barbara Jäger, Marco Stratmann

The framework for photoproduction outlined in Sec. 1.14 can be readily extended to longitudinally polarized ep collisions by replacing all unpolarized hard scattering cross sections and PDFs with their helicity-dependent counterparts. The energy spectrum of circularly polarized photons is given by [225]

$$
\begin{equation*}
\Delta f_{e \gamma}(y)=\frac{\alpha_{e m}}{2 \pi}\left[\frac{1-(1-y)^{2}}{y} \ln \frac{Q_{\max }^{2}(1-y)}{m_{e}^{2} y^{2}}+2 m_{e}^{2} y^{2}\left(\frac{1}{Q_{\max }^{2}}-\frac{1-y}{m_{e}^{2} y^{2}}\right)\right] \tag{1.35}
\end{equation*}
$$

The polarized beams available at an EIC offer unique opportunities for studying the spin structure of circularly polarized photons in photoproduction processes. Such measurements could yield also valuable, complementary information on the gluon helicity density of the proton as we shall demonstrate below.

To study the sensitivity of an EIC to the parton content of polarized photons, which is completely unmeasured so far, we consider two extreme models [226] based on the current knowledge of the unpolarized $f^{\gamma}\left(x, \mu_{0}\right)$ [211] and the positivity constraint $\left|\Delta f^{\gamma}\left(x, \mu_{0}\right)\right| \leq$ $f^{\gamma}\left(x, \mu_{0}\right)$. In the "minimal" scenario we assume $\Delta f^{\gamma}\left(x, \mu_{0}\right)=0$ at a scale $\mu_{0} \simeq 1 \mathrm{GeV}$ and we saturate the bound in the "maximal" scenario, i.e., $\Delta f^{\gamma}\left(x, \mu_{0}\right)=f^{\gamma}\left(x, \mu_{0}\right)$.

We present results of NLO calculations for single-inclusive jet photoproduction at a c.m.s. energy of $\sqrt{s}=100 \mathrm{GeV}$. In order to compute the cross section for jet production, an algorithm has to be specified describing the formation of jets by the final-state partons produced in the hard scattering. A frequently adopted choice is to define a jet as the deposition of the total transverse energy of all final-state partons that fulfill $\left(\eta-\eta^{i}\right)^{2}+$ $\left(\phi-\phi^{i}\right)^{2} \leq R^{2}$, where $\eta^{i}$ and $\phi^{i}$ denote the pseudo-rapidities and azimuthal angles of the particles and $R$ the jet cone aperture. We work in the so-called "small-cone approximation" [227, 228, 229, 230, 231] which can be considered as an expansion of the jet cross section in terms of $R$ of the form $A \log R+B+\mathcal{O}\left(R^{2}\right)$. Neglecting $\mathcal{O}\left(R^{2}\right)$ pieces, the evaluation and phase-space integration of the partonic cross sections can be performed analytically. This approximation has been shown [231, [232, 233, 147] to account extremely well for jet observables up to cone sizes of about $R \approx 0.7$ in related $p p$-scattering reactions by explicit comparison to calculations that take $R$ fully into account.

Figure 1.50 presents our results 234 for the expected NLO double-spin asymmetry $A_{L L}^{j e t}$ for single-inclusive jet photoproduction at $\sqrt{S}=100 \mathrm{GeV}$ for two different choices of proton helicity densities [24, 25] and the two extreme sets of polarized photon densities introduced above. In (1.35) we chose $Q_{\max }^{2}=1 \mathrm{GeV}^{2}$ and the range of photon energies is limited to $0.2 \leq y \leq 0.85$; see also Sec. 1.14. The jet transverse momentum is integrated over for $p_{T}>4 \mathrm{GeV}$, and the factorization and renormalization scales are chosen to be $p_{T}$.

For single-inclusive observables, the rapidity-differential cross sections and the spin asymmetry are particularly interesting, since the relevant ranges of momentum fractions of the partons in the photon and the proton are related to the rapidity of the observed jet. As explained, e.g., in Ref. [235], if counting positive rapidity in the forward direction of the proton, large momentum fractions $x_{\gamma} \simeq 1$ are probed at large negative values of $\eta$. In this region, the direct contribution is expected to be largest and the photon structure is dominated by the purely perturbative "pointlike" QED part [226] which does not depend on the unknown non-perturbative input. As can be seen in Fig. 1.50, measurements of $A_{L L}^{j e t}$


Figure 1.50. Pseudo-rapidity dependence of the NLO QCD spin asymmetry for single-inclusive jet photoproduction at $\sqrt{S}=100 \mathrm{GeV}$ integrated over $p_{T}>4 \mathrm{GeV}$ for two different choices of proton helicity PDFs and two extreme sets of polarized photon densities. Taken from Ref. [234].
for negative $\eta$ can provide valuable information on the proton's spin structure, in particular, the gluon helicity density due to the dominance of gluon-induced processes. On the other hand, at large positive rapidities, $A_{L L}^{j e t}$ is particularly sensitive to the parton content of the resolved photon, $x_{\gamma} \ll 1$, as is also exemplified in the figure. The size of $A_{L L}^{j e t}$ increases if the lower cut for the jet transverse momentum is raised to larger values. The range in $p_{T}$ where jets can be reliably reconstructed at an EIC still needs to be investigated in detail.

If one has determined the proton helicity PDFs from elsewhere, see Sec. 1.11, the prospects for learning about the parton content of polarized photons are excellent. We note that the latter may become relevant in estimates of photon induced cross sections at a future linear collider if the lepton beams will be longitudinally polarized. Resolved photon contributions also complicate current extractions of $\Delta g(x, \mu)$ in polarized-lepton nucleon scattering experiments at fixed-target energies [236, 237]. We have estimated the expected size of statistical uncertainties in case of the related single-inclusive pion photoproduction at an EIC in Ref. [238]. Measurements appear to be feasible already with very moderate integrated luminosities of a few $\mathrm{fb}^{-1}$ thanks to the sizable cross sections for small $Q^{2}$.

We note that other promising observables, like di-jet production where one has a better control of the range of $x_{\gamma}$ probed, see Sec. 1.14, or heavy quark production still need to be studied. Some theoretical results and simulations, mainly for HERA energies, can be found in Refs. [235, 239, 225].

## Chapter 2

# Three-dimensional structure of the proton and nuclei: transverse momentum 

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### 2.1 Introduction and chapter summary

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The exploration of the internal structure of the nucleon in terms of quarks and gluons, the fundamental degrees of freedom of Quantum Chromodynamics (QCD), has been and still is at the frontier of hadronic high energy physics research. After four decades of Deep Inelastic Scattering (DIS) experiments of high energy leptons off nucleons, our knowledge of the nucleon structure has made impressive progress. To leading order in the electromagnetic coupling constant $\alpha_{\text {QED }} \sim \frac{1}{137}$ the lepton with initial momentum $l$ interacts via one photon exchange with the quarks inside the nucleon. By observing the momentum $l^{\prime}$ of the lepton in the final state one obtains information about the quark and gluon content of the nucleon.

This information is encoded in the Parton Distribution Function (PDF) $f_{1}^{a}\left(x, Q^{2}\right)$ where $x=Q^{2} /(2 P \cdot q)$ is the fraction of the nucleon momentum $P$ which is carried by the parton with $Q^{2}=-q^{2}$ and $q=l-l^{\prime}$. This PDF can be interpreted as the number density of partons of type $q$ inside the nucleon, carrying a momentum fraction $x$. Similar information has been obtained about the number density of longitudinally polarized partons inside longitudinally polarized nucleons, the helicity distribution $g_{1}^{a}\left(x, Q^{2}\right)$. The successful prediction of the scale $\left(Q^{2}\right)$ dependence of the PDFs is one of the great triumphs of QCD.

However consolidated our understanding of the nucleon structure from DIS experiments is, it is basically one-dimensional. From DIS we 'only' learn about the longitudinal motion of partons in a fast moving nucleon or, which is equivalent, about their momentum distributions along the light-cone direction singled out by the hard momentum flow in the process (i.e., in DIS, of the virtual photon). In DIS the nucleon is seen as a bunch of fast-moving quarks, antiquarks and gluons, whose transverse momenta are not resolved. A fast moving nucleon is Lorentz-contracted but its transverse size is still about 1 fm , which is a large distance on the strong interaction scale.

It makes therefore sense to ask questions like: how are quarks spatially distributed inside the nucleon? How do they move in the transverse plane? Do they orbit, and carry orbital angular momentum? Is there a correlation between orbital motion of quarks, their spin and the spin of the nucleon? How can we access information on such spin-orbit correlations, and what will this tell us about the nucleon? Recent theoretical progress has put many of these questions on a firm field-theoretical basis. We do not know all answers, yet, but we have now a much better idea on how to get them. The past decade has also witnessed tremendous experimental achievements which lead to fascinating new phenomenological insights into the structure of the nucleon.

The above questions address two complementary aspects of the nucleon structure: the description of quarks in the transverse plane in momentum space and in coordinate space. The field-theoretical tools adequate to describe the former are the Transverse Momentum Dependent Parton Distribution Functions (TMD PDFs, or, shortly, TMDs). The fieldtheoretical objects tailored to describe the spatial distributions of quarks in the transverse plane are the Generalized Parton Distributions (GPDs), which are discussed in chapter 3.1. The focus of this chapter is on the TMDs, their theoretical properties and phenomenological implications.

Several fascinating topics are related to the study of TMDs:

- 3D-imaging. The TMDs depend on the intrinsic motion of partons inside the nucleon and allow the reconstruction of the nucleon structure in momentum space. Such an
information, when combined with the analogous information on the parton spatial distribution from GPDs, leads to a complete 3-dimensional imaging of the nucleon.
- Orbital motion. Most TMDs would vanish in the absence of parton orbital angular momentum. The possibility of learning about the orbital motion of quarks inside a nucleon emerges from the study of TMDs.
- Spin-orbit correlations. Most TMDs and related, observable, azimuthal asymmetries, are due to couplings of the transverse momentum of quarks with the nucleon (or the quark) spin. Spin-orbit correlations, similar to those in hydrogen atoms, can therefore be studied.
- QCD gauge invariance and universality. The origin of some TMDs and the related spin asymmetries, when considered at partonic level, reveal fundamental properties of QCD, mainly its color gauge invariance. This interpretation leads to expect some clear differences, between TMDs, in different processes (universality breaking). A test of such ideas is crucial for our understanding of QCD at work.


### 2.1.1 What are TMDs?

The 'simplest' TMD is the unpolarized function $f_{1}^{q}\left(x, k_{\perp}\right)$ which describes, in a fast moving nucleon, the probability to find a quark carrying the longitudinal momentum fraction $x$ of the nucleon momentum, and a transverse momentum $k_{\perp}=\left|\boldsymbol{k}_{\perp}\right|$. It is formally related to the collinear ('integrated') PDF by $\int \mathrm{d}^{2} \boldsymbol{k}_{\perp} f_{1}^{q}\left(x, k_{\perp}\right)=f_{1}^{q}(x)$ (notice that, for brevity, the dependence of TMDs and PDFs on auxiliary scales is often not indicated).

This and other quark TMDs are defined in terms of the unintegrated quark-quark correlator [240, 241]

$$
\begin{equation*}
\Phi_{i j}^{q}\left(x, \boldsymbol{k}_{\perp}, \boldsymbol{S}\right)_{\eta}=\left.\int \frac{d z^{-} d^{2} z_{\perp}}{(2 \pi)^{3}} \mathrm{e}^{i k \cdot z}\langle\boldsymbol{P}, \boldsymbol{S}| \bar{\psi}_{j}^{q}(0) \mathcal{W}_{\eta}(0, z) \psi_{i}^{q}(z)|\boldsymbol{P}, \boldsymbol{S}\rangle\right|_{z^{+}=0} \tag{2.1}
\end{equation*}
$$

in which the gauge link operator $\mathcal{W}_{\eta}(0, z)$ ensures the color gauge invariance of the matrix element. $\mathcal{W}_{\eta}(0, z)$ depends on a path. Factorization theorems give the prescription along which path the positions 0 and $z$ of the quark fields have to be connected, and the index $\eta$ indicates that strictly speaking $\mathcal{W}_{\eta}(0, z)$ depends on the process, as it will be further discussed. The light-cone coordinates are defined as $a^{\mu}=\left(a^{-}, a^{+}, \boldsymbol{a}_{\perp}\right)$ with $a^{ \pm}=\frac{1}{\sqrt{2}}\left(a^{0} \pm\right.$ $\left.a^{3}\right)$ and $\boldsymbol{a}_{\perp}=\left(a^{1}, a^{2}\right)$.

The power and rich possibilities of the TMD approach arise from the simple fact that $\boldsymbol{k}_{\perp}$ is a vector, which allows various correlations with the other vectors involved: the nucleon momentum $\boldsymbol{P}$ and the nucleon spin $\boldsymbol{S}$. A systematic description of the information content of the correlator was initiated in [242, 243, 244]. Of particular importance are 'leading-twist' TMDs, i.e. TMDs which enter in observables without power suppression. In this context, a TMD or observable is said to be twist-t if its contribution to a cross section is suppressed by the factor $(M / Q)^{t-2}$ [245] in addition to kinematic overall factors ( $M$ represents a generic hadronic scale including the transverse momentum.).

The leading-twist TMDs are associated with the large + component of the nucleon momentum (in a frame where the nucleon moves fast). For a spin $\frac{1}{2}$ particle like the nucleon there are 8 leading-twist TMDs, namely (we suppress the $\eta$ process dependence
label)

$$
\begin{align*}
\frac{1}{2} \operatorname{tr}\left[\gamma^{+} \Phi^{q}\left(x, \boldsymbol{k}_{\perp}, \boldsymbol{S}\right)\right] & =f_{1}^{q}\left(x, k_{\perp}\right)-\frac{\varepsilon^{j k} k_{\perp}^{j} S_{T}^{k}}{M} f_{1 T}^{\perp q}\left(x, k_{\perp}\right)  \tag{2.2}\\
\frac{1}{2} \operatorname{tr}\left[\gamma^{+} \gamma_{5} \Phi^{q}\left(x, \boldsymbol{k}_{\perp}, \boldsymbol{S}\right)\right] & =S_{L} g_{1 L}^{q}\left(x, k_{\perp}\right)+\frac{\boldsymbol{k}_{\perp} \cdot \boldsymbol{S}_{T}}{M} g_{1 T}^{q}\left(x, k_{\perp}\right)  \tag{2.3}\\
\frac{1}{2} \operatorname{tr}\left[i \sigma^{j+} \gamma_{5} \Phi^{q}\left(x, \boldsymbol{k}_{\perp}, \boldsymbol{S}\right)\right] & =S_{T}^{j} h_{1}^{q}\left(x, k_{\perp}\right)+S_{L} \frac{k_{\perp}^{j}}{M} h_{1 L}^{\perp q}\left(x, k_{\perp}\right) \\
& +\frac{\left(k_{\perp}^{j} k_{\perp}^{k}-\frac{1}{2} \boldsymbol{k}_{\perp}^{2} \delta^{j k}\right) S_{T}^{k}}{M^{2}} h_{1 T}^{\perp q}\left(x, k_{\perp}\right)+\frac{\varepsilon^{j k} k_{\perp}^{k}}{M} h_{1}^{\perp q}\left(x, k_{\perp}\right)(2.4)
\end{align*}
$$

Dirac structures other than those above yield higher twist TMDs [246, 247]. TMDs of antiquarks and gluons are defined similarly in terms of correlators analogous to (2.1). The notation used in Eqs. (2.2)-(2.4) follows [243, 244, 245], where the common subscript 1 is used to indicate twist-2 TMDs. (Notice that in the TMD literature also a different notation is often used, in which, for instance, $\Delta^{N} f_{q / p^{\uparrow}}\left(x, k_{\perp}\right)=-\left(2 k_{\perp} / M\right) f_{1 T}^{\perp q}\left(x, k_{\perp}\right)$. We refer to [248] for an overview.)

The leading twist TMDs (2.2 (2.4) have partonic interpretations. The gamma-structures signal the quark polarizations. $\gamma^{+}$describes unpolarized quarks, thus Eq. (2.2) gives the number density of unpolarized quarks inside an unpolarized (first term) or transversely polarized (second term) proton. $\gamma^{+} \gamma_{5}$, which appears in Eq. (2.3), singles out longitudinally polarized quarks, either in a longitudinally (first term) or transversely polarized (second term) proton. Finally, in Eq. (2.4), the gamma-factor $i \sigma^{+j} \gamma_{5}$ selects transversely polarized quarks inside transversely polarized (first and third terms), longitudinally polarized (second term) or unpolarized (fourth term) protons.

### 2.1.2 Partonic interpretation and properties of the TMDs

As they are the central focus of interest in this Chapter, let us further elaborate on the leading order TMDs and their partonic interpretation. We also introduce the Transverse Momentum Dependent Fragmentation Functions (TMD FFs). The TMDs contain information on the longitudinal and transverse (or intrinsic) motion of quarks and gluons inside a fast moving nucleon. When adding the spin degree of freedom they link the parton spin (say a quark, $\boldsymbol{s}_{q}$ ) to the parent proton $\operatorname{spin}(\boldsymbol{S})$ and to the intrinsic motion $\left(\boldsymbol{k}_{\perp}\right)$. The correlator (2.1) restricted to leading twist defines the most general spin dependent TMD, which we denote by $f_{1}^{q}\left(x, \boldsymbol{k}_{\perp} ; \boldsymbol{s}_{q}, \boldsymbol{S}\right)$, and may depend on all possible combinations of the pseudo-vectors $\boldsymbol{s}_{q}, \boldsymbol{S}$ and the vectors $\boldsymbol{k}_{\perp}, \boldsymbol{P}$ which are allowed by parity invariance. At leading order in $1 / Q$, there are eight such combinations, leading to the eight independent TMDs in Eqs. (2.2/2.4).

A similar correlation between spin and transverse motion can occur in the fragmentation process of a transversely polarized quark, with spin vector $\boldsymbol{s}_{q}$ and three-momentum $\boldsymbol{k}_{q}$, into a hadron with longitudinal momentum fraction $z$ and transverse momentum $\boldsymbol{P}_{\perp}$ (with respect to the quark direction); such a mechanism is called the Collins effect [249] and appears in the fragmentation function via a $\boldsymbol{s}_{q} \cdot\left(\boldsymbol{k}_{q} \times \boldsymbol{P}_{\perp}\right)$ term. For a quark fragmentation into a spinless hadron there are two independent leading-twist transverse momentum dependent fragmentation functions.

We briefly list here the eight leading-twist Transverse Momentum Dependent Partonic Distributions of a proton and the two Fragmentation Functions (for a final spinless hadron),
which are the main objects in our investigation of the nucleon momentum structure.

- $f_{1}^{a}\left(x, k_{\perp}\right)$ is the unpolarized, $k_{\perp}$ dependent distribution of parton $a$ inside a proton. Its integrated version is the usual PDF measured in DIS. Common notations are $q(x)=\int d^{2} \boldsymbol{k}_{\perp} f_{1}^{q}\left(x, k_{\perp}\right)$, and $g(x)=\int d^{2} \boldsymbol{k}_{\perp} f_{1}^{g}\left(x, k_{\perp}\right)$ for quarks of flavor $q$ and gluons respectively.
Most experimental and theoretical efforts have so far been dedicated to $q\left(x, Q^{2}\right)$ and $g\left(x, Q^{2}\right)$; these are by now the best known partonic distributions, and the comparison of the predicted $Q^{2}$ dependence with data has been a great success for perturbative QCD.
- $g_{1 L}^{a}\left(x, k_{\perp}\right)$ (or simply $g_{1}^{a}$ ) is the unintegrated helicity distribution: the difference between the number density of partons $a$ with the same and opposite helicity of the parent proton. Common notations for the integrated helicity distributions are $\Delta q(x)=\int d^{2} \boldsymbol{k}_{\perp} g_{1 L}^{q}\left(x, k_{\perp}\right)$ for quarks and similarly $\Delta g(x)$ for gluons. See the relevant discussions in section 1.10 .
The $\Delta q(x)$ 's are not so well known as the corresponding $q(x)$, as they require polarized DIS, but have been measured by several experiments. The least known of the helicity distributions is the gluon one, $\Delta g(x)$, despite some attempts to measure it.
- $h_{1}^{q}\left(x, k_{\perp}\right)$ is the analogue of the helicity distribution, for transverse nucleon spin, i.e. the transversity distribution. The integrated version has several notations in the literature $\Delta_{\perp} q(x)=h_{1}^{q}(x)=\int d^{2} \boldsymbol{k}_{\perp} h_{1}^{q}\left(x, k_{\perp}\right)$ for quarks of flavor $q$. There is no transversity distribution for gluons in a spin $\frac{1}{2}$ hadron.
The unpolarized, the helicity and the transversity distributions are the only three independent PDFs which survive in the collinear limit, $\boldsymbol{k}_{\perp}=0$. The transversity distribution is chiral-odd and needs to be coupled to another chiral-odd quantity to be observed. So far only one extraction of the $u$ and $d$ quark transversities is available in the literature [250], obtained by a combined fit of SIDIS and $e^{+} e^{-}$data.
A good knowledge of the transversity distributions for quarks and antiquarks would allow computation of the tensor charge, given by $\int_{0}^{1} d x\left[h_{1}^{q}(x)-h_{1}^{\bar{q}}(x)\right]$, a non perturbative quantity for which lattice and model computations exist.
- $f_{1 T}^{\perp a}\left(x, k_{\perp}\right)$ is the Sivers function [251, appearing in the distribution of unpolarized partons $a$ inside a polarized proton. It links the parton intrinsic motion to the proton spin:

$$
\begin{equation*}
f_{1}^{a}\left(x, \boldsymbol{k}_{\perp} ; \boldsymbol{S}\right)=f_{1}^{a}\left(x, k_{\perp}\right)-\frac{k_{\perp}}{M} f_{1 T}^{\perp a}\left(x, k_{\perp}\right) \boldsymbol{S} \cdot\left(\hat{\boldsymbol{P}} \times \hat{\boldsymbol{k}}_{\perp}\right) . \tag{2.5}
\end{equation*}
$$

The Sivers function offers new information and plays a crucial role in our understanding of the nucleon structure. Its observation, already confirmed, is a clear indication of parton orbital motion; the opposite values for $u$ and $d$ quarks is argued to be linked to the nucleons' anomalous magnetic moments; its very origin and expected process dependence are related to fundamental QCD effects. Due to its importance the Sivers TMD for quarks will be discussed at length in Sec. 2.2 and for gluons in Sec. 2.3, Theoretical issues concerning $f_{1 T}^{\perp a}$, its origin and relation with basic QCD properties like the color gauge links and color gauge invariance will be treated in Sec. [2.4.

- $h_{1}^{\perp q}\left(x, k_{\perp}\right)$ is the Boer-Mulders function [244, appearing in the distribution of polarized quarks $q$ inside an unpolarized proton:

$$
\begin{equation*}
f_{1}^{q}\left(x, \boldsymbol{k}_{\perp} ; \boldsymbol{s}_{q}\right)=\frac{1}{2} f_{1}^{q}\left(x, k_{\perp}\right)-\frac{k_{\perp}}{2 M} h_{1}^{\perp q}\left(x, k_{\perp}\right) \boldsymbol{s}_{q} \cdot\left(\hat{\boldsymbol{P}} \times \hat{\boldsymbol{k}}_{\perp}\right) . \tag{2.6}
\end{equation*}
$$

This function has the striking peculiarity that it might give unexpected spin effects even in unpolarized processes, as it singles out polarized quarks from unpolarized protons and neutrons. It will be discussed in Sec. 2.5.

- The remaining three TMDs, $g_{1 T}^{a}\left(x, k_{\perp}\right), h_{1 L}^{\perp q}\left(x, k_{\perp}\right)$ and $h_{1 T}^{\perp q}\left(x, k_{\perp}\right)$ are related to double spin correlations in the PDFs; respectively, the amount of longitudinally polarized partons in a transversely polarized proton, of transversely polarized quarks in a longitudinally polarized proton, and of transversely polarized quarks in a transversely (but in a different direction) polarized proton. Neglecting higher-twist terms, some approximate relationships with the other TMDs can be obtained [252]. They will briefly be discussed in Sec. 2.6,
- $D_{1}^{a}\left(z, P_{\perp}\right)$ (also denoted as $D_{h / a}$ ) is the unpolarized, $P_{\perp}$ dependent, parton $a$ fragmentation function (into a hadron $h$ ). Its integrated version $D_{1 h}^{a}(z)=\int d^{2} \boldsymbol{P}_{\perp} D_{1}^{a}\left(z, P_{\perp}\right)$ is the usual FF.
- $H_{1}^{\perp q}\left(z, P_{\perp}\right)$ is the Collins function [249], describing the fragmentation of a polarized quark into a spinless (or unpolarized) hadron:

$$
\begin{equation*}
D_{1}^{q}\left(z, \boldsymbol{P}_{\perp} ; \boldsymbol{s}_{q}\right)=D_{1}^{q}\left(z, P_{\perp}\right)+\frac{P_{\perp}}{z M_{h}} H_{1}^{\perp q}\left(z, P_{\perp}\right) \boldsymbol{s}_{q} \cdot\left(\hat{\boldsymbol{p}}_{q} \times \hat{\boldsymbol{P}}_{\perp}\right) \tag{2.7}
\end{equation*}
$$

The Collins effect has been observed by several experiments and is well established. It is considered as a universal property of the quark hadronization process and it plays a crucial role in many spin effects. Its chiral-odd nature makes it the ideal partner to access chiral-odd TMDs like the transversity distribution and the Boer-Mulders function. All these will be discussed in Sec. 2.5.

### 2.1.3 How do we obtain information on TMDs?

Our guiding experiments involve again lepton-nucleon scattering at high energy, with the difference, with respect to the usual DIS, that one observes in the final state a hadron in addition to the scattered lepton, $\ell(l)+N(P) \rightarrow \ell\left(l^{\prime}\right)+h\left(P_{h}\right)+X$, the so-called SemiInclusive Deep-Inelastic Scattering (SIDIS). In this case the hadron, which results from the fragmentation of a scattered quark, 'remembers' the original motion of the quark, including the transverse one, and offers new information.

In general, SIDIS depends on six kinematic variables. In addition to the variables for inclusive DIS, $x, y=(P \cdot q) /(P \cdot l)$, and the azimuthal angle $\phi_{S}$ describing the orientation of the target spin vector for transverse polarization, one has three variables for the final state hadron, which we denote by $z=\left(P \cdot P_{h}\right) /(P \cdot q)$ (longitudinal hadron momentum), $P_{h T}$ (magnitude of transverse hadron momentum), and the angle $\phi_{h}$ for the orientation of $\boldsymbol{P}_{h T}$ (see also Fig. 2.1). In the one-photon exchange approximation, the SIDIS cross section can be decomposed in terms of structure functions [242, 247, 254, 255] where, largely following


Figure 2.1. Illustration of the kinematics, especially the azimuthal angles, for SIDIS in the target rest frame [253. $\boldsymbol{P}_{h T}$ and $\boldsymbol{S}_{T}$ are the transverse parts of $\boldsymbol{P}_{h}$ and $\boldsymbol{S}$ with respect to the virtual photon momentum $\boldsymbol{q}=\boldsymbol{l}-\boldsymbol{l}^{\prime}$.
the notation of [247], one has

$$
\begin{align*}
\frac{d \sigma}{d x_{B} d y d \phi_{S} d z_{h} d \phi_{h} d P_{h T}^{2}} \propto & \left\{F_{U U, T}+\varepsilon \cos \left(2 \phi_{h}\right) F_{U U}^{\cos 2 \phi_{h}}\right. \\
& +S_{\|} \varepsilon \sin \left(2 \phi_{h}\right) F_{U L}^{\sin 2 \phi_{h}}+S_{\|} \lambda_{\ell} \sqrt{1-\varepsilon^{2}} F_{L L} \\
+ & \left|S_{\perp}\right|\left[\sin \left(\phi_{h}-\phi_{S}\right) F_{U T, T}^{\sin \left(\phi_{h}-\phi_{S}\right)}+\varepsilon \sin \left(\phi_{h}+\phi_{S}\right) F_{U T}^{\sin \left(\phi_{h}+\phi_{S}\right)}\right. \\
& \left.\quad+\varepsilon \sin \left(3 \phi_{h}-\phi_{S}\right) F_{U T}^{\sin \left(3 \phi_{h}-\phi_{S}\right)}\right] \\
& \left.+\left|\boldsymbol{S}_{\perp}\right| \lambda_{e} \sqrt{1-\varepsilon^{2}} \cos \left(\phi_{h}-\phi_{S}\right) F_{L T}^{\cos \left(\phi_{h}-\phi_{S}\right)}+\ldots\right\} \tag{2.8}
\end{align*}
$$

In Eq. (2.8), $\varepsilon$ is the degree of longitudinal polarization of the virtual photon which can be expressed through $y$ [247], $S_{\|}$denotes longitudinal target polarization, and $\lambda_{e}$ is the lepton helicity. The structure functions $F_{X Y}(X$ and $Y$ refer to the lepton and the nucleon, respectively: $U=$ unpolarized; $L, T=$ longitudinally, transversely polarized) merely depend on $x, z$, and $P_{h T}$. The third subscript $F_{X Y, T}$ specifies the polarization of the virtual photon. By choosing specific polarization states and weighting with the appropriate azimuthal dependence, one can extract each structure function in (2.8) as pioneering experiments have already unambiguously shown.

For TMD studies one is interested in the kinematic region defined by

$$
\begin{equation*}
P_{h T} \simeq \Lambda_{\mathrm{QCD}} \ll Q \tag{2.9}
\end{equation*}
$$

for which the structure functions can be written as certain convolutions of TMDs. In this region, the components in Eq. (2.8) appear at leading order when expanding the cross section in powers of $1 / Q$, while additional ones show up at sub-leading order [242, 247, 254, 255]. Measuring the structure functions in Eq. (2.8) allows one to obtain information on all eight leading quark TMDs. To be specific, one has (for a spinless final state hadron) [247, 255],

$$
\begin{array}{ll}
F_{U U} \sim \sum_{q} e_{q}^{2} f_{1}^{q} \otimes D_{1}^{q} & F_{L T}^{\cos \left(\phi-\phi_{S}\right)} \sim \sum_{q} e_{q}^{2} g_{1 T}^{q} \otimes D_{1}^{q} \\
F_{L L} \sim \sum_{q} e_{q}^{2} g_{1 L}^{q} \otimes D_{1}^{q} & F_{U T}^{\sin \left(\phi-\phi_{S}\right)} \sim \sum_{q} e_{q}^{2} f_{1 T}^{\perp q} \otimes D_{1}^{q} \\
F_{U U}^{\cos (2 \phi)} \sim \sum_{q} e_{q}^{2} h_{1}^{\perp q} \otimes H_{1}^{\perp q} & F_{U T}^{\sin \left(\phi+\phi_{S}\right)} \sim \sum_{q} e_{q}^{2} h_{1 T}^{q} \otimes H_{1}^{\perp q} \tag{2.12}
\end{array}
$$

$$
\begin{equation*}
F_{U L}^{\sin (2 \phi)} \sim \sum_{q} e_{q}^{2} h_{1 L}^{\perp q} \otimes H_{1}^{\perp q} \quad F_{U T}^{\sin \left(3 \phi-\phi_{S}\right)} \sim \sum_{q} e_{q}^{2} h_{1 T}^{\perp q} \otimes H_{1}^{\perp q} \tag{2.13}
\end{equation*}
$$

where $e_{q}$ is the charge of the struck quark in units of the elementary charge. Notice that the four chiral-even TMDs couple to the well known unpolarized fragmentation function $D_{1}$, while the chiral-odd TMDs couple to the (chiral-odd) Collins function $H_{1}^{\perp}$. In the subsequent sections the major focus will be on $F_{U T}^{\sin \left(\phi-\phi_{S}\right)}$ containing the Sivers function.

The factorized expressions for the structure functions in Eqs. (2.10) -(2.13) hold in this form in the parton model approximation. If loop corrections are included, one not only obtains a nontrivial higher order term describing the hard scattering part of the process but also a leading-twist contribution arising from soft gluon emission (soft factor) [240, 256, 257, 258, 259, 260. In the case of inclusive DIS such soft gluon effects cancel between real and virtual radiative corrections, but they survive in the SIDIS cross section for $P_{h T} \simeq \Lambda_{\mathrm{QCD}}$. While the hard coefficient enters the structure functions in a simple multiplicative way, the soft factor gets convoluted with the parton distributions and the fragmentation functions. The presence of uncanceled soft gluon emission also requires to somewhat generalize the field-theoretical definition of TMDs given above. More details about this point will be presented in Sec. 2.4.

Almost all existing analyses of TMD-observables are based on the parton model approximation. This is sufficient for getting a good first idea about the general features of the TMDs and also at the present stage of the data, which often are plagued by considerable uncertainties. However, precision studies will be necessary to reveal features of QCD dynamics. The parton model approach will then be no longer appropriate, and one will have to deal with soft gluon effects, especially when high quality data from the EIC become available that will cover a large kinematic range.

### 2.1.4 Gauge invariance, universality, and beyond

Local gauge invariance is the underlying principle of the Standard Model of Particle Physics. In the case of QCD it is the $\mathrm{SU}(3)$ gauge invariance associated with the color degree of freedom of the quarks which matters. This color gauge invariance plays a particularly crucial role for TMDs. Here a brief introduction to this topic is given, while especially in Sec. 2.4 more details about this very active and fascinating field can be found.

As discussed in Sec. 2.1.1, in order to have a gauge invariant definition of TMDs a gauge link (Wilson line) has to be inserted between the two quark fields showing up in the correlator in Eq. (2.1). This is not specific for TMDs but applies also to, e.g., ordinary PDFs. However, two features are unique in the case of TMDs: first, certain TMDs are non-zero only if the Wilson line is taken into account [261, 262, 263, 264]. Second, the Wilson line depends on the process, which leads to a nontrivial universality behavior of TMDs [262].

The mere existence of two TMDs depends on the presence of the Wilson line - the Sivers function $f_{1 T}^{\perp}$ and the Boer-Mulders function $h_{1}^{\perp}$. They are also denoted as naive timereversal odd (T-odd) functions. (This term is not related to real violation of T-invariance but, roughly speaking, is associated with a nontrivial phase at the amplitude level of a process.)

The Wilson line is automatically generated when carrying out factorization. In the case of SIDIS, it arises due to the exchange of (infinitely many) gluons between the active struck quark and the remnants of the target. Since in DIS these exchanges happen after the
virtual photon strikes the quark one also talks about final state interactions (FSI). On the other hand, for the Drell-Yan process, there exist corresponding gluon exchanges before the photon-quark interaction, which we call initial state interactions (ISI). As a consequence, the Wilson-lines for the two processes are running along different paths. This in turn endangers the universality (process-independence) of TMDs, which is a crucial prerequisite for factorization being of any practical use.

Although the paths of the Wilson lines are different, the TMDs for both processes can be related by using the parity and time-reversal transformation [262. One finds that the six T-even TMDs are actually universal, while the T-odd TMDs are non-universal. However, this non-universality is well under control and 'merely' consists of a sign change [262],

$$
\begin{equation*}
\left.f_{1 T}^{\perp}\right|_{\text {DY }}=-\left.f_{1 T}^{\perp}\right|_{\text {DIS }},\left.\quad h_{1}^{\perp}\right|_{\text {DY }}=-\left.h_{1}^{\perp}\right|_{\text {DIS }} \tag{2.14}
\end{equation*}
$$

In other words, the predictive power of factorization is maintained. The experimental check of this sign change is currently one of the outstanding topics in hadronic physics.

We are now in a position to further motivate why the study of the Sivers effect should play a central role in the EIC science case. First, the Sivers function not only tells us something about the three-dimensional structure of the nucleon, a particular spin-orbit correlation, etc. Its physics is also intimately related to the gauge invariance of QCD. Second, existing data for non-zero transverse single-spin asymmetries in SIDIS and in proton-proton collisions can be explained on the basis of the Sivers effect. In other words, the physics of FSI/ISI is the key to describing these asymmetries (which can be as large as $40 \%$ ) in QCD. Third, according to our present knowledge, in SIDIS the Sivers function is easier to measure than the Boer-Mulders function. Fourth, the check of the predicted sign reversal in (2.14), strictly speaking, is more direct for $f_{1 T}^{\perp}$ than for the chiral-odd $h_{1}^{\perp}$. In the latter case input from models is required.

Quite some progress was made in recent years to further elucidate this physics associated with the underlying gauge structure of QCD. In particular, for hadron-hadron collisions with hadronic final states the presence of both ISI and FSI may unable any kind of (standard) TMD-factorization [265, 266, 267, 268, 269, 270, 271, 272. The consequences of a breakdown of TMD-factorization are far-reaching. For instance, in such a case also the so-called QCD resummation technique [273], which is widely used whenever there is more than one physical momentum scale in a process, becomes questionable. Moreover, if the sign reversal of the Sivers function in Eq. (2.14) is not confirmed by experiment, the general procedure of applying QCD to hard scattering processes may have to be revisited. Further striking developments in this rather new field can be expected, and only the close interplay between lepton-nucleon scattering and hadronic collisions will allow us to fully explore this physics, as is also obvious from the relations (2.14).

### 2.1.5 TMDs and orbital angular momentum

The helicity PDFs $g_{1}^{a}(x)$ are still not well known, especially in the sea quark and gluon sector, but by now one fact seems clear: the spin of quarks and gluons accounts only for a part of the nucleon spin. A substantial fraction of the nucleon spin must be due to orbital angular momentum (OAM). It is important to keep in mind that in gauge theories there is no unique decomposition of the nucleon spin into contributions due to the spin and OAM of quarks and gluons [143, 274]. Nevertheless it is possible [274, 275] to learn about OAM from GPDs which describe the dynamics of partons in the transverse plane in position space.

TMDs provide complementary information on the dynamics of partons in the transverse plane in momentum space, and one naturally expects TMDs to teach us about parton OAM. That the OAM of partons plays an important role is well known: in the light-cone wave function of the nucleon components with OAM $L_{z} \neq 0$ must be present in order to have a non-zero anomalous magnetic moment [276, 277], and the situation is similar for several other quantities [278]. Model calculations have also shown that the leading twist TMDs $f_{1 T}^{\perp q}, g_{1 T}^{q}, h_{1}^{\perp q}, h_{1 L}^{\perp q}, h_{1 T}^{\perp q}$ and many sub-leading twist TMDs would vanish without different components in the nucleon wave function with $\Delta L_{z} \neq 0$. But although OAM seems to play a crucial role also for many TMDs, so far no rigorous connection between the OAM contribution of partons and the nucleon spin could be established.

### 2.1.6 Further important topics

In this subsection some further important aspects about TMDs are briefly discussed; more details will be presented in the other Sections of this TMD Chapter.

## Models and lattice QCD

Model calculations have had a particularly strong impact on the TMD field. It suffices to recall the calculations in the quark-diquark model [261] which helped to establish the existence of the Sivers effect within QCD and the TMD factorization framework [262]. Models may allow to see more clearly the relevant aspects of TMDs which are obscured in the much more complicated QCD dynamics. We encountered one promising instance of that above, in Sec. 2.1.5. Model results have, however, also very practical applications. Nearly nothing is known about most of the TMDs. Models provide information on the sign and magnitude of TMDs, or possible (model) relations among different TMDs. This information can be applied to make predictions for the planned experiments, and in this way help to better explore the opportunities of the available and planned facilities. The importance of model studies is discussed in Sec. 2.4

Lattice QCD is in principle a powerful approach. What can be handled presently in lattice studies are calculations of the matrix element in the integrand of the correlator in Eq. (2.1), i.e., TMDs in Fourier-space. Most readily accessible is information on $x$-integrated TMDs such as $\int d x f_{1}^{q}\left(x, k_{\perp}\right)$ [279, 280]. The caveat is that lattice results presently available have been obtained with a simplified gauge-link in the correlator (2.1). This simplified gauge-link differs from the link-geometry dictated by factorization in a particular scattering process. Investigations with more realistic gauge-links are ongoing.

## Gluon TMDs

In addition to the eight TMDs for quarks, there also exist eight TMDs for gluons [248, 281, 282. The most prominent one is the unpolarized gluon TMD, which is a widely used ingredient of many calculations in high-energy processes. Because of the initial and final state interactions, the universality of this object is nontrivial and has attracted renewed interest lately [283]. Moreover, linearly polarized gluons for an unpolarized nucleon can, in principle, be explored through, e.g., heavy quark pair production in $\ell p$-collisions [284]. A particularly important role is played by the Sivers function for gluons, which will be discussed in quite some detail in Sec. 2.3. Experimentally, the sector of gluon TMDs is largely unexplored so far, and the EIC could provide extremely valuable information in this respect.

## Moments of TMDs

Momentum moments of some of the TMDs are of particular interest because of their relation to certain collinear 3-parton correlators, which appear in the QCD-description of, e.g., SIDIS structure functions at large $P_{h T} \simeq Q$ or weighted asymmetries (see Sec. 2.2). For instance, in the case of the Sivers function one can consider the moment [264, 285]

$$
\begin{equation*}
f_{1 T}^{\perp(1)}(x) \equiv \int d^{2} \boldsymbol{k}_{\perp} \frac{\boldsymbol{k}_{\perp}^{2}}{2 M^{2}} f_{1 T}^{\perp}\left(x, \boldsymbol{k}_{\perp}^{2}\right)=\pi T_{F}(x, x) \tag{2.15}
\end{equation*}
$$

where $T_{F}$ represents a quark-gluon-quark correlator. These correlation functions were also introduced in the literature to describe the single-spin asymmetries in hard scattering processes in the collinear factorization framework [286, 287, 288, 289]. Equation (2.15) is a model-independent result which allows one to relate different observables. A corresponding relation holds for the Boer-Mulders function [264, 285]. Also the moments $g_{1 T}^{(1)}$ and $h_{1 L}^{\perp(1)}$ can be expressed through collinear 3-parton correlators [290].

## Integrated/weighted observables

In Sec. 2.1.3 leading-twist soft gluon effects were mentioned. Such effects can cancel if the components in Eqs. (2.8) are integrated upon the transverse momentum $P_{h T}$ of the hadron. For instance, a cancellation occurs for the unpolarized structure function $F_{U U}$, and also for the term associated with $F_{U T}^{\sin \left(\phi_{h}-\phi_{S}\right)}$ which is related to the Sivers effect [291]. In the latter case the integration needs to be done with a proper weight factor (a more elaborate account on this topic will be given in Sec. (2.2). Such weighted observables are therefore rather attractive from a theoretical point of view. They depend on moments of the TMDs just discussed above and as such provide additional complementary information. The EIC would be ideal for seriously studying these interesting observables.

## Structure functions from low to high transverse momenta

While at low $P_{h T}$ the SIDIS structure functions can be described by means of TMDfactorization, for $P_{h T} \simeq Q$ collinear factorization is the appropriate framework. Recently, a lot of progress has been made to understand the quantitative relation between TMDfactorization on the one hand and collinear factorization on the other in the region $\Lambda_{\mathrm{QCD}} \ll$ $P_{h T} \ll Q$ where both approaches apply [292, 293, 294, 295, 296, 297]. An extended discussion of these aspects, with a focus on the EIC, will also be given in Sec. 2.2,

## Higher twist TMDs

The focus of present research is on the leading-twist TMDs. However, there is also a lot of important information encoded in twist-3 TMDs, which contain detailed information on the quark-gluon correlators. Experimentally, such twist-3 effects can be explored by measuring sub-leading structure functions appearing in the general decomposition of the SIDIS cross section (2.8) [242, 247, 254, 255]. In fact, the first clear single-spin phenomena in SIDIS, which crucially vitalized the field, were sub-leading twist observables. Although studied in numerous works, these first data on single-spin asymmetries in SIDIS remain basically unexplained. Some aspects of the interesting topic of higher twist TMDs will be discussed in more detail in Sec. 2.6.

| Deliverables | Observables | What we learn | Phase I | Phase II |
| :---: | :---: | :---: | :---: | :---: |
| Sivers + unp. | SIDIS with Tran. | Quant. Interf. | valence+sea | 3D Imaging of |
| TMD quarks | polarization/ion; | Multi-parton \& | quarks, overlap | quarks \& gluon; |
| and gluon | di-hadron (di-jet) | Spin-Orbit | with the fixed | $Q^{2}\left(P_{\perp}\right)$ range |
|  | heavy flavor | correlations | target exp. | QCD dynamics |
| Chiral-odd | SIDIS with Tran. | $3^{\text {rd }}$ basic quark | valence+sea | $Q^{2}\left(P_{\perp}\right)$ range |
| functions: | polarization/ion; | PDF; novel | quarks, overlap | for detailed |
| Transversity; | di-hadron | hadronization | with the fixed | QCD dynamics |
| Boer-Mulders | production | effects | target exp. |  |

Table 2.1. Science Matrix for TMD physics: 3D structure in transverse momentum space: golden measurements (upper part) and silver measurements (lower part).

### 2.1.7 TMDs and the EIC

Despite the tremendous progress in understanding TMDs and the related physics, without a new lepton-hadron collider many aspects of this fascinating field will remain untouched or at least on a qualitative level. Existing facilities either suffer from a much too restricted kinematic coverage or from low luminosity or from both. Based on the present status of research we see the following potential in an EIC:

- clean quantitative measurements of TMDs in the valence region due to high luminosity, and ability to go to sufficiently large $Q^{2}$ in order to suppress potential higher twist contaminations. Primordial orbital motion is expected for valence quarks.
- related to the wide kinematic coverage and the high luminosity, ability to provide multi-dimensional representations of the observables, which is basically impossible on the basis of current experiments.
- production and possible observation of jets with significantly larger particle multiplicities, allowing for the study a larger variety of hadronic final states.
- first access to TMDs for antiquarks.
- (first) access to TMDs for gluons, for instance through dihadron correlations, dijet correlations, or semi-inclusive production of quarkonium.
- systematic study of perturbative QCD techniques (for polarization observables). Tests and studies of QCD evolution properties of TMDs.

We strongly believe that the EIC will bring our knowledge of the partonic structure of the nucleon to an entirely new level. Keeping in mind deeply QCD rooted effects, like the (potential) sign-change of the Sivers function, the EIC can be expected to stimulate further developments in the application of perturbative QCD to other hard scattering processes. A series of "golden" and "silver" measurements are outlined in table 2.1. The significance of these points is further enhanced by newly planned (polarized) Drell-Yan experiments, which will study complementary physics aspects.

### 2.2 Sivers function

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We choose the example of the Sivers function to illustrate the physics case for TMD distributions at the EIC. This function incorporates all new facets and intriguing physical aspects of TMD distributions outlined in the introduction and discussed in more detail in the following sections. We start this discussion with a brief review of the peculiarities of the Sivers function thereby illustrating the crucial role TMDs play in our understanding of the nucleon structure.

The Sivers function $f_{1 T}^{\perp a}\left(x, k_{\perp}\right)$, appearing in the distribution of unpolarized partons $a$ inside a polarized nucleon:

$$
\begin{equation*}
f_{1}^{a}\left(x, \boldsymbol{k}_{\perp} ; \boldsymbol{S}\right)=f_{1}^{a}\left(x, k_{\perp}\right)-\frac{k_{\perp}}{M} f_{1 T}^{\perp a}\left(x, k_{\perp}\right) \boldsymbol{S} \cdot\left(\hat{\boldsymbol{P}} \times \hat{\boldsymbol{k}}_{\perp}\right) \tag{2.16}
\end{equation*}
$$

describes the correlation between the momentum direction of the struck parton and the spin of its parent nucleon and is hence related to the orbital motion of partons inside the nucleon. This correlation generates a dipole pattern in the transverse $k_{\perp}$-plane. We illustrate this fascinating aspect of certain TMDs in providing a three-dimensional imaging of the nucleon in momentum space by choosing a specific configuration for the vectors involved in Eq. (2.16). Taking for example $\hat{\boldsymbol{P}} \equiv \frac{\mathbf{P}}{|\mathbf{P}|}=(0,0,-1)$ and the spin of the proton along the $y$ direction, so that $S=(0,1,0)$ and the transverse momentum of the parton $k_{\perp}=\left(k_{\perp x}, k_{\perp y}, 0\right)$, yields a typical "dipole" modulation of the distribution:

$$
\begin{equation*}
f_{1}^{a}\left(x, \boldsymbol{k}_{\perp} ; \boldsymbol{S}\right)=f_{1}^{a}\left(x, k_{\perp}\right)+\frac{k_{\perp x}}{M} f_{1 T}^{\perp a}\left(x, k_{\perp}\right) \tag{2.17}
\end{equation*}
$$

The $f_{1}$ term provides an axially symmetric contribution, while the second term containing $f_{1 T}^{\perp}$ gives rise to the dipole pattern. A superposition of both effects results in a distribution that is shifted away from the center (distorted) in the $k_{\perp}$-plane as shown in fig. 2.2. This distortion turns out to be of opposite sign for up and down quarks.

The Sivers function manifests the importance of initial and final state interaction effects in hard scattering processes as the presence of these effects is required for the existence of a non-zero Sivers function. Their inclusion in the TMD factorization approach yields a peculiar breaking of the universality of the Sivers function. As introduced in sec. 2.1.4 and detailed in sec. 2.4.1, this non-universality is well under control and 'merely' consists of a sign change of the Sivers function when appearing in the Drell-Yan process as compared to DIS. The experimental verification of this sign change is currently one of the outstanding topics in hadronic physics and presents a crucial test for our understanding of hadron production in high-energy reactions. We will therefore briefly review the prospects for measurements of the Sivers effect in Drell-Yan in sec. 2.2.3.

A further intriguing aspects of the Sivers function is its connection to the orbital angular momentum in the nucleon. A non-zero quark Sivers function involves a transition between initial and final nucleon states that differ by one unit of orbital angular momentum. This property together with the potential for a three-dimensional imaging, puts the Sivers function in close relation to the GPD $E$ discussed in chapter 3. In particular, it was proposed that there is a dynamical relation called "chromodynamic lensing", where


Figure 2.2. Spin density in the transverse-momentum plane for unpolarized quarks in a transversely polarized nucleon, as described by the Sivers function. The left panel is for up quarks and the right one for down quarks. The model calculation of Ref. [298] was used.
the spatial distortion of the transverse quark distribution (in a transversely polarized proton) leads to a distortion in transverse momentum distribution described by the Sivers function [299, 300, 301].

### 2.2.1 What do we know so far from experiments?

Though the Sivers function was first suggested to explain the surprisingly large singlespin asymmetries measured in $p p$ collisions, our guiding experiments for obtaining unambiguous information about this function, and most of the other TMDs, involve high-energy lepton-nucleon scattering with the observation of one or more hadrons in coincidence with the scattered lepton (semi-inclusive DIS). In addition, model calculations of TMDs, discussed in sec. 2.4. guide Ansätze for global fits of TMD parameterizations and provide an interpretation of the various aspects of TMDs.

In this section, after a brief review of the results from $p p$ collisions, we will summarize available semi-inclusive DIS measurements of observables related to the Sivers effect and present phenomenological extractions of the Sivers function from data. The following section will then highlight the potential of an EIC for a detailed and systematic exploration of the various aspects of the quark Sivers functions illustrative of TMDs in general.

## Transverse-spin effects in proton-proton collisions

Historically, the surprisingly large left-right asymmetries observed in hadronic reactions with transversely polarized protons initiated the idea about a transverse momentum dependence of quark distributions in polarized protons. The pioneering measurements 302, 303] of these large (up to 0.3-0.4 in magnitude) transverse-spin asymmetries in inclusive forward production of pions in $p p$ collisions $p^{\uparrow} p \rightarrow \pi+X$, have been extensively confirmed by experiments at FermiLab [304, 305, 306, 307, 308] and at RHIC (BNL) at much higher center-of-mass energies of up to $\sqrt{s}=200 \mathrm{GeV}$ [309]. The observation of such asymmetries was frequently quoted as a puzzle or challenge for theory. In fact, for a long time, transverse single-spin asymmetries were assumed to be negligible in hard scattering processes [310].

The work of [251] introduced a transverse momentum dependent quark distribution, now termed the Sivers function, which provides a mechanism for the observed asymmetries that does not vanish at high energies.

A rich variety of single-spin asymmetries for identified hadrons $\left(\pi^{ \pm}, \pi^{0}, K^{ \pm}, p, \bar{p}\right)$ measured over a wide kinematic range is now available from the BRAHMS, PHENIX and STAR experiments at RHIC (BNL) [311, 312, 313, 314, 315, 316, 317, 318. The results exhibit a general pattern: sizable asymmetries are measured at forward-rapidity and for positive Feynman $x_{F}>0.3$ which increase in magnitude with increasing $x_{F}$ and $P_{h T}$. In contrast, for negative $x_{F}$ and at mid-rapidity all asymmetries are found to be consistent with zero.

Several mechanisms have been suggested to explain these asymmetries. At large values of $P_{h T}$ collinear factorization involving twist-3 distributions can be applied. However, the intrinsic prediction of a $1 / P_{h T}$ fall-off has yet to be confirmed. An alternative approach using a generalized parton model that takes intrinsic transverse momentum dependences into account has been used to describe existing data, achieving a fairly successful description of the observed asymmetries for pion production in $p p$ collisions 319. If less inclusive measurements are performed, with an observed soft momentum scale in addition to a hard scale, one can attempt to describe the data using a TMD approach in pQCD. However, as discussed in sec. 2.4.1, the presence of both initial and final state interactions in hadronhadron collisions may prevent any kind of (standard) TMD-factorization. More insight might be gained regarding the intricate color structure of $p p$ reactions for example by measuring di-jet production. In di-jet production both large scales (e.g., jet $p_{T}$ ) and small scales (e.g., $\Delta p_{T}$ of nearly back-to-back jets) can be observed. To assess factorization breaking due to color interactions in $p p$ collisions, the experimental measurements can be compared to calculations using TMDs extracted from DIS and Drell-Yan, for which TMDfactorization has been demonstrated. Little experimental information currently exists on these processes, but they are part of the physics program at RHIC.

Many questions still need to be answered, but it is clear that for a strict assessment of whether the TMD Ansatz is indeed possible and appropriate to describe results from hadronic collisions, more precise parameterizations of the Sivers function and, hence, more precise data on the Sivers effect in a well-understood process like DIS is needed.

## Semi-inclusive Deep-Inelastic Scattering

In semi-inclusive DIS, the Sivers function leads to single-spin asymmetries in the distribution of hadrons in the azimuthal angles illustrated in fig. [2.1. The azimuthal modulations of the SIDIS cross section are given in Eq. (2.8). The Sivers effect manifests itself as a $\sin \left(\phi_{h}-\phi_{S}\right)$ modulation and requires transverse polarization of the target nucleon. The additional information provided by the azimuthal angle $\phi_{S}$ of the transverse component of the target-proton spin about the virtual photon direction allows for an unambiguous extraction of the Sivers effect. Experimentally, the so-called Sivers amplitude $2\left\langle\sin \left(\phi_{h}-\phi_{S}\right)\right\rangle_{U T}^{h}$ [253], which projects out the structure function $F_{U T, T}^{\sin \left(\phi_{h}-\phi_{S}\right)}$ in Eq. (2.8) for a specific hadron $h$, is extracted from the asymmetry

$$
\begin{equation*}
A_{U T}^{h}\left(\phi_{h}, \phi_{S}\right) \equiv \frac{1}{\left|\mathbf{S}_{T}\right|} \frac{d \sigma^{h}\left(\phi_{h}, \phi_{S}\right)-d \sigma^{h}\left(\phi_{h}, \phi_{S}+\pi\right)}{d \sigma^{h}\left(\phi_{h}, \phi_{S}\right)+d \sigma^{h}\left(\phi_{h}, \phi_{S}+\pi\right)}, \tag{2.18}
\end{equation*}
$$

where the subscript $U$ indicates an unpolarized lepton beam and $T$ a transversely polarized target nucleon. This amplitude has so far been extracted by three polarized fixed-target experiments as summarized in Tab.[2.2. From these measurements, fig. [2.3]shows a selection

| experiment (laboratory) | $\sqrt{s}$ in GeV | target type | hadron types | references |
| :--- | :---: | :---: | :---: | :---: |
| COMPASS (CERN) | 18 | deuteron | $h^{ \pm}, \pi^{ \pm}, K^{ \pm}, K^{0}$ | $[320,321]$ |
|  |  | proton | $h^{ \pm}$ | $[322$ |
|  |  | proton | $\pi^{ \pm}, K^{ \pm}$ | prelim. 323 |
| HERMES (DESY) | 7.4 | proton | $\pi^{ \pm}$ | $[324$ |
|  |  | proton | $\pi^{ \pm},\left(\pi^{+}-\pi^{-}\right), \pi^{0}, K^{ \pm}$ | $[325]$ |
| HallA (JLab) | 3.5 | neutron | $\pi^{ \pm}$ | prelim. [326] |

Table 2.2. Summary of currently available measurements of Sivers asymmetry amplitudes from lepton-nucleon DIS experiments, their center-of-mass energy, transversely polarized target type, and analyzed hadron types.
of results that are significantly non-zero and help in determining the shape of the Sivers function. All other asymmetry amplitudes listed in Tab. 2.2 are small or consistent with zero.

The results have so far been interpreted in the parton model as a convolution of distribution and fragmentation functions, where the Sivers amplitude can be approximated by

$$
\begin{equation*}
2\left\langle\sin \left(\phi_{h}-\phi_{S}\right)\right\rangle_{U T}^{h}\left(x_{B}, y, z_{h}, P_{h T}\right)=-\frac{\sum_{q} e_{q}^{2} f_{1 T}^{\perp q}\left(x, k_{\perp}^{2}\right) \otimes_{\mathcal{W}} D_{1}^{q}\left(z, P_{\perp}^{2}\right)}{\sum_{q} e_{q}^{2} f_{1}^{q}\left(x, k_{\perp}^{2}\right) \otimes D_{1}^{q}\left(z, P_{\perp}^{2}\right)} \tag{2.19}
\end{equation*}
$$

Here the sums run over the quark flavors, the $e_{q}$ are the quark charges, and $f_{1}\left(x, k_{\perp}^{2}\right)$ and $D_{1}\left(z, P_{\perp}^{2}\right)$ are the spin-independent quark distribution and fragmentation functions, respectively. The symbol $\otimes\left(\otimes_{\mathcal{W}}\right)$ represents a (weighted) convolution integral over intrinsic and fragmentation transverse momenta, $\boldsymbol{k}_{\perp}$ and $\boldsymbol{P}_{\perp}$ respectively, as explicitely given in (2.21).

A qualitative picture of the Sivers function can already be derived from the measured asymmetry amplitudes. The non-zero results shown in fig. 2.3 are obtained with a proton target. As scattering off $u$ quarks dominates these data due to the charge factor, the positive Sivers amplitudes for $\pi^{+}$and $K^{+}$suggest a large and negative Sivers function for up quarks. This is supported by the positive amplitudes of the pion difference asymmetry, which originates mainly from the difference $\left(f_{1 T}^{\perp d_{v}}-4 f_{1 T}^{\perp u_{v}}\right)$ in the Sivers functions for valence down and up quarks and is dominated by the contribution from valence $u$ quarks. The vanishing amplitudes for $\pi^{-}$require cancellation effects, e.g. from a $d$ quark Sivers function opposite in sign to the $u$ quark Sivers function. Such cancellation effects between Sivers functions for up and down quarks are supported by the vanishing asymmetry amplitudes extracted from deuteron data by the COMPASS collaboration. An interesting facet of the data shown in fig. 2.3 is the magnitude of the $K^{+}$amplitudes, which are nearly twice as large as those of the $\pi^{+}$. Again, on the basis of $u$ quark dominance, one might naively expect that the $\pi^{+}$and $K^{+}$amplitudes should be similar. Their difference in size may thus point to a significant role of other quark flavors, e.g. sea quarks.

Phenomenological analyses of HERMES and COMPASS data [327, 328, 329, 330, 331, 332 , confirm the picture drawn above as discussed in the following. So far, only the analysis of Ref. [327] makes use of a subset of the most recent data listed in Tab. 2.2 and all fits have yet to be updated for the results from proton data from COMPASS and the first neutron data from HallA.


Figure 2.3. Sivers amplitudes for $\pi^{+}, K^{+}$and the pion-difference (as denoted in the panels) from HERMES 325 and for $\pi^{+}$and $K^{+}$from COMPASS 323] measured with a proton target. Inner error bars present statistical uncertainties and full error bars the quadratic sum of statistical and systematic uncertainties. Note that the average kinematics in each bin differs for HERMES and COMPASS.

## Phenomenological extractions and models of the Sivers function

The strong impact and success of model calculations and lattice QCD on the TMD field is discussed in detail in sec. 2.4 and sec. 4.1. respectively. Models provide information on the magnitudes and signs of TMDs and guide Ansätze for global fits of TMD parameterizations. For example, from chiral models [333] and the QCD limit of a large number of colours (large $N_{c}$ limit) [334] a Sivers function for up and down quarks of equal size but with opposite $\operatorname{sign}\left(f_{1 T}^{\perp u}=-f_{1 T}^{\perp d}\right)$ is predicted.

Phenomenological analyses provide extractions of TMDs from data. As discussed in sec. 2.1.3, existing analyses of TMD observables are so far based on the parton model approximation, where the measured amplitudes of the SIDIS cross section in Eq. (2.8), are expressed as convolutions of distribution $f^{q}$ and fragmentation functions $D^{q}$. For the Sivers amplitude it reads

$$
\begin{equation*}
F_{U T, T}^{\sin \left(\phi_{h}-\phi_{S}\right)} \propto \sum_{q} e_{q}^{2} f_{1 T}^{\perp q}\left(x, k_{\perp}^{2}\right) \otimes \mathcal{W} D_{1}^{q}\left(z, P_{\perp}^{2}\right) \tag{2.20}
\end{equation*}
$$

where $\otimes \mathcal{W}$ is defined as

$$
\begin{equation*}
\otimes_{\mathcal{W}} \equiv \int d^{2} \boldsymbol{k}_{\perp} d^{2} \boldsymbol{P}_{\perp} \delta^{(2)}\left(z \boldsymbol{k}_{\perp}+\boldsymbol{P}_{\perp}-\boldsymbol{P}_{h T}\right) \mathcal{W} \tag{2.21}
\end{equation*}
$$

with the kinematic factor $\mathcal{W}$ depending on the involved transverse momenta. This convolution can be resolved by either employing a particular model for the transverse momentum


Figure 2.4. Up and down quark Sivers distributions extracted from HERMES (and for the full line also from COMPASS) data using three different parameterizations [329, 330, 331] (see text). The left and right panels show, respectively, the first and the $1 / 2$ moment. The curves indicate the 1 -sigma regions of the various parameterizations. None of three parameterizations makes use of the latest experimental results listed in Tab. 2.2,
dependence or by integrating over the transverse momentum $P_{h T}$ using a proper weight factor in the extraction of the asymmetry amplitudes which involves $P_{h T}$, building for example $2\left\langle\frac{P_{h T}}{M_{p}} \sin \left(\phi_{h}-\phi_{S}\right)\right\rangle_{U T}^{h}$. The latter approach is very attractive but experimentally challenging for measurements at current fixed target facilities as it requires full $P_{h T}$ coverage, which cannot be obtained at any of the existing experiments. An EIC would be the ideal facility to study such weighted asymmetries and to seriously explore the advantages of these observables, as further discussed in sec. 2.2.7.

An intuitive and common Ansatz for the transverse momentum dependence of distribution and fragmentation functions, which provides an analytic solution of (2.21), is a Gaussian distribution like

$$
\begin{equation*}
f_{1 T}^{\perp q}\left(x, k_{\perp}^{2}\right)=f_{1 T}^{\perp q}(x) \frac{1}{\pi\left\langle k_{\perp}^{2}\right\rangle} \exp \left(-\frac{\boldsymbol{k}_{\perp}^{2}}{\left\langle k_{\perp}^{2}\right\rangle}\right), \quad D_{1}^{q}\left(z, P_{\perp}^{2}\right)=D_{1}^{q}(z) \frac{1}{\pi\left\langle P_{\perp}^{2}\right\rangle} \exp \left(-\frac{\boldsymbol{P}_{\perp}^{2}}{\left\langle P_{\perp}^{2}\right\rangle}\right) \tag{2.22}
\end{equation*}
$$

with typical values for $\left\langle k_{\perp}^{2}\right\rangle$ and $\left\langle P_{\perp}^{2}\right\rangle$ of 0.2 to $0.3 \mathrm{GeV}^{2}$.
The Sivers function was among the first to be extracted from data, as it couples to the usual unpolarized fragmentation function $D_{1}^{q}$. This fragmentation function is reasonably well parameterized [335, 336] using precise data from electron-positron annihilation into charged hadrons and, most recently, also from single-hadron production in $p p$ collisions and semi-inclusive DIS [74], which provide complementary information on the flavour dependence of the fragmentation process.

Figure 2.4 shows the extraction of the up and down quark Sivers distributions using three different parameterizations for the Sivers function [329, 330, 331, presenting $k_{\perp}-$ moments defined as

$$
\begin{equation*}
f^{(1)}(x) \equiv \int d^{2} \boldsymbol{k}_{\perp} \frac{\boldsymbol{k}_{\perp}^{2}}{2 M^{2}} f\left(x, k_{\perp}^{2}\right) \quad \text { and } \quad f^{(1 / 2)}(x) \equiv \int d^{2} \boldsymbol{k}_{\perp} \frac{\left|\boldsymbol{k}_{\perp}\right|}{2 M} f\left(x, k_{\perp}^{2}\right) . \tag{2.23}
\end{equation*}
$$

The parameterization from Ref. [329] (full line) is based on a combined fit to previous HERMES and COMPASS data, while the other two fit HERMES data only but describe


Figure 2.5. The Sivers function for $u$ quarks extracted from recent experimental data 327. Vertical lines indicate the region where experimental data are available. The band represents the 2 -sigma range for the chosen parameterization. The dashed blue lines indicate the positivity bound.
the COMPASS data well when using the obtained parameters to calculate the asymmetries for COMPASS kinematics. All three extractions use the parameterization from Ref. [335] for the unpolarized fragmentation function. The two curves of each set indicate the 1-sigma regions of the various parameterizations, taking into account solely statistical uncertainties of the data sets employed in the fit. The three approaches describe the HERMES Sivers asymmetries equally well. The differences in size and shape of the extracted Sivers up and down quark distributions hence reflect the model dependence of the fit results. The parameterization of 331 imposes the constraint from the large $N_{c}$ limit, which results in the symmetric parametrization of up and down Sivers distributions, shown in the left panel of fig. 2.4 with dashed lines. None of the extractions involve parameterizations for sea quarks as they could not be constrained by the data used in the fits.

However, the recent, surprisingly large, Sivers asymmetry amplitudes for $K^{+}$measured by HERMES, which were found to be nearly twice as large as those of the $\pi^{+}$, might hint at a possibly important role of sea quarks. In Ref. [327], the sensitivity of these data to sea quark contributions was tested. A fit including Sivers functions for only up and down quarks was compared with a second fit that allowed also for sea quark contributions ( $\bar{u}, \bar{d}, s, \bar{s}$ ) to the Sivers amplitude. Both fits describe the data with equally good $\chi^{2}$, demonstrating that their precision is not yet good enough to independently constrain the Sivers function for six quark flavours. In this analysis, the usage of new parameterizations of the fragmentation functions from Ref. [74] was essential for obtaining a good description of the kaon data.

The available parameterizations of the Sivers function for up and down quarks 327, [328, 331, 332 agree, within their large uncertainties, with calculations based on a lightcone model 298 and on a diquark spectator model 337, 338, while predictions based on the bag model [339] appear to be too small in magnitude for both the up and down quark Sivers function (see also sec. 2.4).

## Open issues in extractions of the Sivers function

Figure 2.5 illustrates our current knowledge of the Sivers function. So far, only the up and down quark Sivers functions can be constrained with relatively large uncertainties within the range $0.004<x<0.5$ using basic parameterizations for their shapes.

The precision of current data permits neither constraints of the Sivers functions for
sea quarks nor an employment of more flexible functional forms, which would also allow for a sign change as suggested by a spectator model (see fig. 2.22 in sec. 2.4). The band in fig. [2.5 represents the 2 -sigma range for the chosen parameterization and reflects the precision of the data, but does not account for model uncertainties or for variations of the functional form of the parameterizations. Also not estimated so far, is any uncertainty stemming from the Gaussian Ansatz used to resolve the convolution in (2.21). For example, the average value, $\left\langle k_{\perp}^{2}\right\rangle$, of the quark intrinsic transverse momentum used in this Ansatz might be flavour dependent, and both $\left\langle k_{\perp}^{2}\right\rangle$ and $\left\langle P_{\perp}^{2}\right\rangle$ dependent on the energy scale. The latter is particularly relevant for the fragmentation functions, which are extracted from data collected at much higher energy than the available SIDIS asymmetry data used in the fits. The EIC would provide both TMD observables at substantially higher scale than any fixed target DIS experiment and unique data sets of hadron production for a flavour tagging in the fragmentation process and a study of its transverse momentum dependence.

At this stage of analysis, also specific known issues of experimental data are ignored. For example, the limited precision of currently available SIDIS data usually allows only for presenting the results as a function of one kinematic variable while integrating over the others within the experimental acceptance. Hence, the asymmetry amplitudes from a specific experiment, presented for different kinematic variables are correlated. Moreover, the experimental acceptance usually does not provide a full coverage in $P_{h T}$. Thus, the 'unweighthed' asymmetry amplitudes extracted as function of $x$ or $z$ present only partial $P_{h T}$ moments in contrast to theoretical considerations. A fully differential analysis of SIDIS data, which requires high statistic datasets, would resolve these issues.

Turning our essentially qualitative picture of the Sivers function and the related physics into a quantitative description, which goes beyond the tree-level approximation, requires new facilities providing high precision polarized data over a wide kinematic range as discussed in the following section.

### 2.2.2 The Sivers function at the EIC

A systematic and detailed study of the Sivers function, and TMDs in general, can only be performed on the basis of precise spin- and azimuthal-asymmetry amplitude measurements in semi-inclusive DIS over a wide kinematic range. The availability of experimental results that are fully differential in the kinematic variables $x, Q^{2}, z$ and $P_{h T}$ would be a great asset for phenomenological analyses, as they permit testing the underlying perturbative QCD techniques and assumptions. Particle identification over the full momentum range and measurements with both proton and (effective) neutron targets would allow for a full flavour separation of the distribution functions under study.

Planned experiments at the upcoming JLab12 facility aim at providing high precision semi-inclusive DIS data in the valence quark region at relatively low $Q^{2}$, taken with transversely polarized neutrons (HallA) [340, protons and deuterons (CLAS12) 341. The expected high luminosities should allow for fully differential extractions of the relevant azimuthal and transverse-spin asymmetries. The kinematic range of JLab12 experiments will be complementary to COMPASS measurements [342], partially overlap with those of HERMES, and provide data in the so-far unexplored high- $x$ region.

The kinematic coverage of these experiments is compared in fig. 2.6 with the coverage of an EIC for an energy setting of $\sqrt{s}=50 \mathrm{GeV}$. As discussed in sec. 7.1]and sec. [7.2, the ability to vary the energy of both the electron and proton (ion) beams at the EIC provides variable energy in the range $\sqrt{s}=15-65 \mathrm{GeV}$ or $\sqrt{s}=45-200 \mathrm{GeV}$ depending on the realization


Figure 2.6. [color online] Kinematic coverage in $x$ and $Q^{2}$ for the EIC for an energy setting of $\sqrt{s}=50 \mathrm{GeV}$ compared to the coverage of COMPASS, HERMES and future JLab12 experiments represented by the red, purple and black hatched areas, respectively.
options under discussion. This ability puts the EIC in the unique position of accessing the valence region at much larger $Q^{2}$ than current and near-future experiments (thereby suppressing potential higher twist contaminations) while also accessing low $x$ down to values of about $10^{-5}$, where sea quarks and gluons could be studied in detail. The expected high luminosity will allow for a fully differential analysis over almost the whole wide kinematic range. In this section we will illustrate this potential for fully differential analyses of TMD observables and test the sensitivity to sea quark distributions. The unique features of the EIC for access to TMDs for gluons, a study of the evolution properties of TMDs, and of the transition from low to high transverse momenta will be discussed, using the Sivers function as an example, in secs. 2.3, 2.4.2 and 2.2.5, respectively.

## Generation of pseudo-data

The projections presented in the following for the Sivers asymmetry where estimated using either modified existing Monte Carlo generators or standard parameterizations of the unpolarized parton distribution and fragmentation functions. Events were generated for $Q^{2}>1 \mathrm{GeV}^{2}, 0.01<y<0.9$ and $0.1<z<0.9$, over the full kinematically allowed range in $x$. At this stage no cuts were applied on the scattered electron or produced hadron. Events were divided into four-dimensional $\left(x, Q^{2}, z, P_{h T}\right)$ bins and the mean asymmetry in each bin was evaluated. Full acceptance in azimuth was assumed and statistical uncertainties of $\sqrt{2 / N}$ were assigned in each bin. More details about the simulations can be found in 343. For all projections shown in the following, no losses due to detector acceptance were applied, but an overall operational efficiency of $50 \%$ was assumed. The transverse proton beam polarization is set to $70 \%$. No estimate of systematic uncertainties is applied.

Most of the projections will be given for an integrated luminosity of $4 \mathrm{fb}^{-1}$ or $30 \mathrm{fb}^{-1}$. These statistics would be achieved in approximately one week to one month ( $4 \mathrm{fb}^{-1}$ ) or


Figure 2.7. Projected accuracy for $\pi^{+}$production in semi-inclusive DIS off the proton for a particular $P_{h T}$ and $z$ range as indicated in the figure. The position of each point is according to its $Q^{2}$ and $x$ value, within the range $0.05<y<0.9$. The projected event rate, represented by the error bar, is scaled to the (arbitrarily chosen) asymmetry value at the right axis. The blue squares, black triangles and red dots represent the $\sqrt{s}=140 \mathrm{GeV}, \sqrt{s}=50 \mathrm{GeV}$ and $\sqrt{s}=15 \mathrm{GeV}$ EIC configurations, respectively. Event counts correspond to an integrated luminosity of $30 \mathrm{fb}^{-1}$ for each of the three configurations.
one month to six month ( $30 \mathrm{fb}^{-1}$ ) for luminosities ranging from $1 \times 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ to $3 \times$ $10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. Therefore the statistical precision in the figures presented here should be understood as that achievable in a relatively brief period of operation for an EIC.

## Four-dimensional mapping of the phase space

The great potential of the EIC for obtaining a fully differential mapping of almost the entire phase space relevant for TMD studies is illustrated in figs. 2.7 and 2.8. A wide $x$ and $Q^{2}$ range can be mapped using different beam energies. The projected accuracy for single $\pi^{+}$production is given for a four-dimensional binning in the kinematic variables $x$, $Q^{2}, z$ and $P_{h T}$, using three different energy configurations for the EIC $(\sqrt{s}=15,50$ and 140 GeV ) and an integrated luminosity of $30 \mathrm{fb}^{-1}$ for each configuration. Events are selected for $0.05<y<0.9$ and $W^{2}>5 \mathrm{GeV}^{2}$. For a clearer view and explanation of the presented projections, we show in fig. 2.7 one of the panels from fig. 2.8 corresponding to a specific $z$ and $P_{h T}$ range. In both figures, the position of each point is according to its $x$ and $Q^{2}$ value (abscissa and left ordinate, respectively) and each panel is for a specific $z$ and $P_{h T}$ bin as indicated in the figure. The projected event rate is represented by the error bar scaled with respect to the (arbitrarily chosen) asymmetry value given at the right ordinate.

The simulations demonstrate that a four-dimensional mapping of TMD observables for pions over the whole phase space of main interest, meaning $P_{h T}$ values of up to about 1 GeV , could be achieved in about 3-5 month of running for each energy configuration. Kaon rates


Figure 2.8. Four-dimensional representation of the projected accuracy for $\pi^{+}$production in semiinclusive DIS off the proton. Each panel corresponds to a specific $z$ bin with increasing value from left to right and a specific $P_{h T}$ bin with increasing value from top to bottom, with values given in the figure. The position of each point is according to its $Q^{2}$ and $x$ value, within the range $0.05<y<0.9$. The projected event rate, represented by the error bar, is scaled to the (arbitrarily chosen) asymmetry value at the right axis. Blue squares, black triangles and red dots represent the $\sqrt{s}=140 \mathrm{GeV}, \sqrt{s}=50 \mathrm{GeV}$ and $\sqrt{s}=15 \mathrm{GeV}$ EIC configurations, respectively. Event counts correspond to an integrated luminosity of $30 \mathrm{fb}^{-1}$ for each of the three configurations.
are typically a factor $4-5$ lower than those for pions and a similar quality of data can be achieved within a correspondingly longer running time.

The strategy for a full flavour separation of the Sivers distribution, and TMD distributions in general, involves both pion and kaon identification over almost the whole momentum range and measurements with proton and effective neutron targets. For the latter, the usage of polarized ${ }^{3} \mathrm{He}$ ions is foreseen for both EIC concepts. Compared to the projections shown in fig. [2.8, the dilution factor of $1 / 3$ has to be compensated with higher luminosities (respectively longer running times). The resulting different phase space for the neutron measurements compared with the proton case due to the $Z / A$ factor entering the momentum distribution and the expected lower center-of-mass energy (by about $2 / 3$ ) because of the different rigidities of the beams can be compensated to a large extent by using the different beam energy settings.

In addition, valuable and necessary information about the transverse momentum dependence of the fragmentation process will be obtained from the same data using a fully differential extraction of the individual hadron multiplicities.

## Sensitivity to sea quarks

Among the unique features of the EIC is its sensitivity for an exploration of the Sivers function for sea quarks, which are expected to play an important role in the lower $x$ region.


Figure 2.9. Simulated Sivers asymmetry amplitudes for $\pi^{+}$, obtained with an energy of $\sqrt{s}=140$ GeV , as a function of $x$ in bins in $z, P_{h T}$ and for a single bin in $Q^{2}$ as given in the panels. Closed blue (open black) dots correspond to (non-)zero Sivers functions for sea quarks. Error bars represent the projected accuracy corresponding to an integrated luminosity of $4 \mathrm{fb}^{-1}$.

We investigate this sensitivity by generating two sets of events, one with and one without contributions from sea quarks. As the Sivers distribution is essentially unknown, it was parameterized via a constant multiplied by the unpolarized PDF with independent constants for $u, d$ and sea quarks. The Sivers asymmetry is returned by the generator on an event-by-event basis. The unpolarized PDFs of [82] and the fragmentation functions of [74] were used.

In both cases, the same parameterization for up and down quark Sivers functions was used, which were set equal to $25 \%$ of the unpolarized distribution, but with opposite sign, i.e. $f_{1 T}^{\perp u}(x)=-0.25 f_{1}^{u}(x)$ and $f_{1 T}^{\perp d}(x)=0.25 f_{1}^{d}(x)$. In the first data set, the Sivers functions for sea quarks were also set to $25 \%$ of the corresponding unpolarized distribution. In the second data set the sea quark Sivers distributions were fixed to zero. This allowed for a comparison of the case in which the sea quark Sivers function was significant compared to that of the valence quarks with the case of a vanishing sea quark contribution.

Figure 2.9shows the asymmetry amplitudes for $\pi^{+}$, obtained with an energy of $\sqrt{s}=140$ GeV , for a single bin in $Q^{2}$ as a function of $x$, binned in $z$ and $P_{h T}$ as indicated in the panels. Open black dots represent the case of non-zero Sivers functions for sea quarks and closed blue dots the case of vanishing contributions. Error bars correspond to an integrated luminosity of $4 \mathrm{fb}^{-1}$, already yielding sufficient precision to resolve small resulting differences in the asymmetry. Because of their different quark content, kaon production is expected to have a higher sensitivity to sea quark contributions. Figure 2.10 shows the asymmetry amplitudes


Figure 2.10. Simulated Sivers asymmetry amplitudes for $K^{+}$, obtained with an energy of $\sqrt{s}=140$ GeV , as a function of $x$ in bins in $z, P_{h T}$ and for a single bin in $Q^{2}$ as given in the panels. Closed blue (open black) dots correspond to (non-)zero Sivers functions for sea quarks. Error bars represent the projected accuracy corresponding to an integrated luminosity of $4 \mathrm{fb}^{-1}$.
for $K^{+}$where indeed both scenarios are more distinct. As for $\pi^{+}$, the estimate is based on an integrated luminosity of $4 \mathrm{fb}^{-1}$ and obtained with an energy of $\sqrt{s}=140 \mathrm{GeV}$.

The study demonstrates that even a relatively brief running of the EIC provides the potential to distinguish zero and non-zero Sivers functions for sea quarks. Note that these parameterizations are intended not as a prediction of what asymmetries will actually be seen at an EIC, but as an indicator of sensitivity given the expected statistical precision.

## Impact of the EIC

The EIC will be the unique facility for exploring the Sivers function (and TMDs in general) for sea quarks and the gluon, to study the evolution properties of TMD distributions and to investigate experimentally the transition from low to high transverse momenta. As discussed in sec. 2.2.1, our current knowledge is restricted to an essentially qualitative picture of the Sivers function. Available data permit to constrain parameterizations for up and down quarks only, employing relatively simple functional forms.

We illustrate the expected impact of data from the EIC using the parameterization from Ref. [327] as an arbitrarily chosen model of the Sivers function. This parameterization, denoted theor ${ }_{i}=F\left(x_{i}, z_{i}, P_{h T}^{i}, Q_{i}^{2} ; \mathbf{a}_{\mathbf{0}}\right)$ with the $M$ parameters $\mathbf{a}_{\mathbf{0}}=\left\{a_{1}^{0}, \ldots, a_{M}^{0}\right\}$ fitted to


Figure 2.11. [color online] Comparison of the precision (2- $\sigma$ uncertainty) of extractions of the Sivers function for $u$ quarks (left) and $d$ quarks (right) from currently available data [327] (grey band) and from pseudo-data generated for the EIC with energy setting of $\sqrt{s}=45 \mathrm{GeV}$ and an integrated luminosity of $4 \mathrm{fb}^{-1}$ (dark grey band around the red line). The uncertainty estimates are for the specifically chosen underlying functional form (see text for details).
existing data, serves to generate a set of pseudo-data in each kinematic bin $i$

$$
\begin{equation*}
f\left(\text { value }_{i} ; \text { theor }_{i}, \sigma_{i}^{2}\right)=\frac{1}{\sqrt{2 \pi \sigma_{i}^{2}}} e^{-\left(\text {value }_{i}-\text { theor }_{i}\right)^{2} / 2 \sigma_{i}^{2}} \tag{2.24}
\end{equation*}
$$

In each $x_{i}, Q_{i}^{2}, z_{i}$ and $P_{h T}^{i}$ bin, the obtained values, value ${ }_{i}$, for the Sivers function are distributed using a Gaussian smearing with a width $\sigma_{i}$ corresponding to the simulated event rate at an energy of $\sqrt{s}=45 \mathrm{GeV}$ obtained with an integrated luminosity of $4 \mathrm{fb}^{-1}$. For illustration of the obtainable statistical precision the event rate for the production of $\pi^{+}$in semi-inclusive DIS was used.

This new set of pseudo-data was then analysed like the real data in Ref. [327]. Figure 2.11 shows the result for the extraction of the Sivers function for $u$ and $d$ quarks. The central value of $f_{1 T}^{\perp u}$, represented by the red line, follows by construction the underlying model. The 2-sigma uncertainty of this extraction, valid for the specifically chosen functional form, is indicated by the dark grey area, which is hardly seen around the red line. This precision, obtainable with an integrated luminosity of $4 \mathrm{fb}^{-1}$, is compared with the uncertainty of the extraction from existing data, represented by the light grey band and shown before in fig. 2.5.

Remembering that the event rate of the generated pseudo-data is achievable in a brief period of operation for an EIC, the impressive impact of the EIC on studies of TMDs is greatly illustrated.

### 2.2.3 TMDs in Drell-Yan processes

One of the intriguing facets of the Sivers effect is its peculiar breaking of universality, as discussed in secs. 2.1.4 and 2.4. The symmetry properties of QCD require a reversal of sign of the Sivers function when appearing in the Drell-Yan process, the production of dilepton pairs in the collision of two hadrons, as compared to DIS. The important test of this fundamental QCD prediction remains outstanding, its invalidation would have profound consequences for our understanding of high-energy reactions involving hadrons. It is thus


Figure 2.12. The correlation of the quark and antiquark momentum fractions, $x_{1}$ and $x_{2}$, in DrellYan for different rapidity bins in proton-proton collisions at $\sqrt{s}=500 \mathrm{GeV}$.
not surprising to see the Drell-Yan process appear as a milestone measurement in the update for the future spin program at RHIC [344.

The Drell-Yan process with unpolarized hadrons has been studied at numerous fixedtarget experiments [345, 346, 347, 348, 349. There are several proposals for future polarized Drell-Yan measurements, either at fixed-target experiments (CERN, FermiLab, GSI, and J-Parc), but also at colliders (BNL, GSI). So far no measurement exists for Drell-Yan with transverse hadron polarization to isolate the Sivers effect, unlike the case for the related mechanism of the Boer-Mulders function. Being a naive-T-odd distribution the latter also involves a reversal of sign when going from DIS to Drell-Yan. For the BoerMulders function data from the Drell-Yan process exist. In particular the violation of the Lam-Tung relation [350 is a substantial hint of the Boer-Mulders effect, as discussed in sec. 2.5.2. However, being also a chiral-odd distribution, presents an additional challenge for experimental measurements and their interpretation, given that a second, presently poorly constrained, chiral-odd function is needed. In the case of Drell-Yan the other chiralodd function is a second Boer-Mulders function, making it especially tricky to look for the sign change between Drell-Yan and DIS.

Among the proposed measurements of the Sivers effect in Drell-Yan two have timescales of a few years from now. One is an experiment set at IP2 of RHIC (BNL) where transversely polarized "beam" protons will interact with effectively unpolarized "target" protons1 344]. At the COMPASS experiment at CERN it is not the beam-in this case consisting of pions - that will be polarized but the target [342]. This configuration is the theoretically more challenging one of the two as the partonic structure of the pion enters besides the structure of the proton.

The choice of measuring Drell-Yan single-spin asymmetries at a collider like RHIC has various advantages. Among others, the asymmetries depend only weakly on the partonic momentum $x_{2}$ of the (anti)quark in the unpolarized nucleon. When integrated over $x_{2}$ the cross section increases with the center-of-mass energy $\sqrt{s}$ as one can reach lower values of $x_{2}$ where anti-quarks are more abundant. Furthermore, it is easier to differentiate between "forward" and "backward" production at a collider allowing easy access to the valence region of the (transversely polarized) beam nucleon. In fig. 2.12, we show the correlation of the quark and antiquark momentum fractions, $x_{1}$ and $x_{2}$, in the Drell-Yan (DY) process

[^270]

Figure 2.13. Sivers asymmetries for the Drell-Yan process at RHIC, as a function rapidity for $\sqrt{s}=500 \mathrm{GeV} 351$.
for different rapidity bins in proton-proton collisions at $\sqrt{s}=500 \mathrm{GeV}$. The plot assumes an invariant mass range of the DY lepton pair between the $J / \psi$ and the Upsilon. To select DY at masses below the $J / \psi$ and/or at rapidities below 2.0 will be experimentally extremely challenging due to the dominance of the QCD $2 \rightarrow 2$ processes $\left(>10^{8}\right)$. The expected single-spin asymmetry, $A_{N}$, is presented in fig. 2.13 as a function of rapidity, $y$, for $\sqrt{s}=500 \mathrm{GeV}$ and integrated over the range $4 \div 9 \mathrm{GeV}$ in the invariant mass of the di-lepton pair [351]. The estimate makes use of a recent "DIS" Sivers function parameterization from fits to COMPASS and HERMES data 332. Asymmetries of this size should be readily measurable with a limited data set. Nevertheless, one should keep in mind that the change of sign applies to the flavor-dependent Sivers function. For a stringent test of this sign change it is therefore of utter importance not only to measure the Sivers effect in DIS and Drell-Yan, but to perform a flavor-decomposition of the Sivers effect as well. In $p p$ collisions one will be mainly sensitive to the $u$-quark Sivers function due to the charge factor. Using pion beams one can vary the sensitivity to the various quark flavors via the choice of the pion charge as the valence anti-quark flavor in the pion will either be an anti- $u$ or an anti- $d$. This will help in a subsequent flavor decomposition of the Sivers effect in Drell-Yan.

### 2.2.4 Single-spin asymmetry in the collinear factorization: Twist-three mechanism

The quark Sivers function discussed in the last subsection is also closely related to the twist-3 quark-gluon-quark correlation functions in the collinear factorization approach which can generate large single spin asymmetries in hard scattering process, in particular, in inclusive hadron production in $p p$ collisions. The single-transverse spin asymmetry in the process like $p p \rightarrow \pi X$ is among the simplest spin observables in hadronic scattering. One scatters a beam of transversely polarized protons off unpolarized protons and measures the numbers of pions produced to either the left or the right of the plane spanned by the momentum and spin directions of the initial polarized protons. Measurements of single-spin asymmetries in hadronic scattering experiments over the past three decades have shown spectacular results. Large asymmetries of up to several tens of percents were observed at forward (with respect to the polarized initial beam) angles of the produced pion. Despite the
conceptual simplicity of $A_{N}$, the theoretical analysis of single-spin asymmetries in hadronic scattering is remarkably complex. The reason for this is that the asymmetry for a singleinclusive reaction like $p p \rightarrow \pi X$ is power-suppressed as $1 / \ell_{\perp}$ in the hard scale set by the observed large pion transverse momentum. Power-suppressed contributions to hardscattering processes are generally much harder to describe in QCD than leading-twist ones. In the case of the single-spin asymmetry, a complete and consistent framework could be developed [286, 288, 289, 352]. It is based on a collinear factorization theorem at nonleading twist that relates the single-spin cross section to convolutions of twist-three quarkgluon correlation functions for the polarized proton with the usual parton distributions for the unpolarized proton and the pion fragmentation functions, and with hard-scattering functions calculated from an interference of two partonic scattering amplitudes: one with a two-parton initial state and the other with a three-parton initial state.

In the following, we briefly describe the collinear factorization formalism for the twist3 single-spin-dependent cross section in the semi-inclusive deep inelastic scattering, ep $\rightarrow$ $e h X$. This factorization applies when the transverse momentum of the final state hadron is large compared to the non-perturbative scale $\Lambda_{\mathrm{QCD}}$. The usual leading twist spin-average cross section for this process can be schematically written as

$$
\begin{equation*}
d \sigma \sim \sum_{a, b} f_{a}(x, \mu) \otimes D_{h / b}(z, \mu) \otimes \hat{\sigma}^{a b}(x, z, Q, \mu), \tag{2.25}
\end{equation*}
$$

where $f_{a}(x, \mu)$ and $D_{h / b}(z, \mu)(a, b=q, \bar{q}, g)$ are, respectively, the parton density in the nucleon and the fragmentation function for $b \rightarrow h$, convoluted with the hart part $\hat{\sigma}^{a b}$. The twist-3 cross section relevant for SSA in $e p^{\uparrow} \rightarrow e h X$ takes the factorized form,

$$
\begin{align*}
d \sigma^{\mathrm{tw} 3} & \sim \sum_{a, b} G_{a}^{(3)}\left(x_{1}, x_{2}, \mu\right) \otimes D_{h / b}(z, \mu) \otimes \hat{\sigma}_{1}^{a b}\left(x_{1}, x_{2}, z, Q, \mu\right) \\
& +\sum_{a, b} \delta f_{a}(x, \mu) \otimes D_{h / b}^{(3)}\left(z_{1}, z_{2}, \mu\right) \otimes \hat{\sigma}_{2}^{a b}\left(x, z_{1}, z_{2}, Q, \mu\right) \tag{2.26}
\end{align*}
$$

where $\otimes$ represents the appropriate convolution, similarly as the twist-2 factorization formula (2.25), with the relevant momentum fractions $x_{1,2}, z, x, z_{1,2}$ integrated over. $G_{a}^{(3)}\left(x_{1}, x_{2}, \mu\right)$ is the twist-3 distribution function in the transversely-polarized nucleon $p^{\uparrow}$, and $D_{h / b}^{(3)}\left(z_{1}, z_{2}, \mu\right)$ is the twist-3 fragmentation function for the hadron $h$; the latter function is chiral-odd, combined with the chiral-odd transversity distribution $\delta f_{a}(x, \mu)$ for $p^{\uparrow}$. (In the TMD approach, the first term in (2.26) is described in terms of the Sivers function, and the second term is described using the Collins function.) These twist-3 distribution and fragmentation functions describe the multi-parton correlations in the nucleon and in the fragmentation process, respectively, and thus provides us with an opportunity to reveal the more detailed internal structure of hadrons beyond the parton-model picture. Each twist-3 function has its own logarithmic scale dependence, which differs from that of the twist-2 functions; for the corresponding $\mu$-dependence, see section (2.4.3).

For $G_{a}^{(3)}\left(x_{1}, x_{2}, \mu\right)$ with $a=q$ in (2.26), two independent quark-gluon correlation functions, $G_{F}\left(x_{1}, x_{2}\right)$ and $\widetilde{G}_{F}\left(x_{1}, x_{2}\right)$, participate. They are defined as dimensionless, real, Lorentz-scalar functions in terms of nucleon matrix element associated with the gluon field strength tensor $F^{\alpha \beta}$ as well as the quark field $\psi$ on the light-cone 352, 353. Similarly, the twist-3 purely gluonic correlation functions $O\left(x_{1}, x_{2}\right)$ and $N\left(x_{1}, x_{2}\right)$ as $G_{g}^{(3)}\left(x_{1}, x_{2}, \mu\right)$ in (2.26), are defined through the gauge-invariant lightcone correlation of three field-strength
tensors [354. Thus, a complete set of the twist-3 correlation functions in the transverselypolarized nucleon is now provided by $G_{F}\left(x_{1}, x_{2}\right), \widetilde{G}_{F}\left(x_{1}, x_{2}\right), O\left(x_{1}, x_{2}\right)$ and $N\left(x_{1}, x_{2}\right)$, taking into account all symmetry constraints in QCD. We note that the twist-3 correlation functions, $T_{F}\left(x_{1}, x_{2}\right), T_{G}^{(f, d)}(x, x)$, etc., used in the literature [355, 356, 357] can be expressed by the above correlation functions.

Another origin of SSA is in the fragmentation process for the final hadron, as represented in terms of the twist-3 fragmentation function $D_{h / b}^{(3)}\left(z_{1}, z_{2}, \mu\right)$ of (2.26), which is also defined as a multi-parton light-cone correlation function (see [297]).

For SIDIS, ep $\rightarrow e h X$, the large transverse-momentum $P_{h T}$ of the hadron $h$ should come from a perturbative mechanism, i.e. from the recoil from the hard (unobserved) final-state partons. Then, the factorization formula (2.26) is derived in the LO perturbative QCD, manifesting their gauge invariance at the twist-3 level, and a practical procedure to calculate the relevant partonic hard part $\hat{\sigma}_{i}^{a b}$ is provided in [352, 354, 297]: an extra gluon, which emanates from nonperturbative multi-parton correlation and carries the momentum fraction $x_{2}-x_{1}$, participates in the partonic hard scattering. The coupling of this gluon allows an internal propagator in the partonic subprocess to be on-shell, and this produces the required imaginary phase. The results for those partonic subprocesses imply [352, 358, 359,

$$
\begin{aligned}
& \frac{d^{5} \sigma^{\mathrm{tw} 3}}{d x_{B} d Q^{2} d z_{h} d P_{h T}^{2} d \phi_{h}}=\sin \left(\phi_{h}-\phi_{S}\right) F^{\sin \left(\phi_{h}-\phi_{S}\right)}+\sin \left(2 \phi_{h}-\phi_{S}\right) F^{\sin \left(2 \phi_{h}-\phi_{S}\right)} \\
&\left.\quad+\sin \phi_{S} F^{\sin \phi_{S}}+\sin \left(3 \phi_{h}-\phi_{S}\right) F^{\sin \left(3 \phi_{h}-\phi_{S}\right)}+\sin \left(\phi_{h}+\phi_{S}\right) F^{\sin \left(\phi_{h}+\phi_{\phi} \phi_{2}\right.}, 27\right)
\end{aligned}
$$

with the azimuthal angles $\phi_{h}$ and $\phi_{S}$ of $P_{h T}$ and $S_{\perp}$, respectively, measured from the lepton plane; the five azimuthal dependences in (2.26) are similar as those in the TMD approach. Here, each structure function $F^{\sin (\cdots)}$ is expressed in a factorized form, convoluted with $G_{F}(x, x)$ and $d G_{F}(x, x) / d x$. The similar twist-3 effects from $G_{F}$ and $\widetilde{G}_{F}$ have been investigated for SSA in Drell-Yan and direct photon productions, and hadron production in $p p$ collisions.

Charm production in SIDIS and $p p$ collisions is useful to study the twist-2 gluon distributions in the nucleon, since the $c \bar{c}$-pair creation through the photon-gluon or gluon-gluon fusion is their driving subprocess. Likewise, the three-gluon correlation functions can be probed by SSA in these processes. From this point of view, the three-gluon contribution to SSA in $D$-meson production processes, $e p^{\uparrow} \rightarrow e D X$ and $p^{\uparrow} p \rightarrow D X$, have been studied in [356, 357, 354, 360]. For both processes, the twist-3 cross sections for SSA can be derived entirely as the gluonic pole contribution leading to $x_{1}=x_{2}$, and thus receive the contributions $O(x, x), O(x, 0), N(x, x)$ and $N(x, 0)$ (and their derivatives) 354, 360]. The result for $e p^{\uparrow} \rightarrow e D X$ has five azimuthal dependences like in (2.27) [354].

So far, RHIC at BNL reported a significant amount of data of $A_{N}$ for $p^{\uparrow} p \rightarrow h X$ ( $h=\pi, K, \eta, D, J / \Psi)$. Given that the NLO QCD in collinear factorization can provide a reasonable description of the corresponding unpolarized cross section, we expect that one can apply the above twist-3 formalism to analyze the $A_{N}$ data [289, 355, 361]. The complete LO QCD formula for $A_{N}$ from the twist-3 quark-gluon correlation functions to $p^{\uparrow} p \rightarrow h X$ has been derived: It consists of the contribution associated with $G_{F}(x, x)$ and $d G_{F}(x, x) / d x\left(\widetilde{G}_{F}(x, x)=0\right)$ 355, and the contribution 362 associated with $G_{F}(x, 0)$ and $\widetilde{G}_{F}(x, 0)$. Phenomenological analysis of RHIC data shows that both contributions are important, although the main contribution comes from the $G_{F}(x, x)$ contribution [289, 355], the $G_{F}(x, 0)\left(\widetilde{G}_{F}(x, 0)\right)$ contribution also plays an important role, and the combination of both contributions provides a reasonable description of the RHIC data, shedding light on


Figure 2.14. Left: kinematics for $D$-meson events showing the momentum vs. polar angle distribution for the electron and $D$ (or equivalently $\bar{D}$ ) meson in the laboratory frame. Right: Projected accuracy for transverse single-spin asymmetries from single $D$ meson production using an energy of $\sqrt{s}=50 \mathrm{GeV}$ and an integrated luminosity of $370 \mathrm{fb}^{-1}$.
the behavior of $G_{F}$ and $\widetilde{G}_{F}$ 361. There are also some initial efforts to calculate the twist-3 fragmentation contribution to $A_{N}$ 363. Global analysis of RHIC and future EIC data is expected to reveal more details on the role of the multi-parton correlations, including the three-gluon correlation functions.

The potential of the EIC for measuring transverse single-spin asymmetries in charm production is illustrated in fig. 2.14. In the simulation, based on the PYTHIA event generator, the main decay channel for $D$ mesons, $D \rightarrow \pi^{+} K^{-}$, with a branching ratio of $3.8 \pm 0.1 \%$ is investigated. Events are selected for $P_{h T}>1 \mathrm{GeV}$ and $Q^{2}>1 \mathrm{GeV}$ within $0.05<y<0.9$ and $1.86<M_{D}<1.87$. The signal-to-background ratio for the reconstructed $D$ mesons strongly depends on the detector resolution. In this study, we assume a momentum resolution of $0.8 \% \cdot \frac{p}{10 \mathrm{GeV}}$ and a resolution of the polar and azimuthal angles of 0.3 mrad and 1 mrad , respectively. The resulting resolution of the reconstructed invariant mass of the $D$ meson is 1.8 MeV yielding an overall signal-to-background ratio of about 1.6 to 1 . The overall detection efficiency for this triple coincidence process is assumed to be $60 \%$. The polarization of the proton beam is set to $80 \%$.

The projected accuracy for measuring transverse single-spin asymmetries in single $D$ meson production is shown in fig. 2.14 (right) as a function of $z$ for different regions in $Q^{2}$, $x$ and $P_{h T}$, as indicated in the figure, together with model calculations of the asymmetry from Ref. [356]. An energy of $\sqrt{s}=50 \mathrm{GeV}$ and an integrated luminosity of $370 \mathrm{fb}^{-1}$ were used. The study demonstrates a very promising feasibility of extracting observables involving charm production. It will significantly benefit from higher energies up to $\sqrt{s}=200$ GeV .

In summary, the twist-3 collinear factorization framework provides us with a systematic way for describing SSA in the region of large transverse-momentum $P_{h T}$ of the final hadron, and is thus complementary to the TMD description of SSA which is valid in the low $P_{h T}$ region. For the twist-3 distribution functions in the transversely-polarized nucleon, relevant to SSA, there are two independent quark-gluon correlation functions and the two indepen-
dent three-gluon correlation functions, all of which are process-independent. Twist-3 cross section formulae for SSA are available for many important processes, which can be used for confronting with the RHIC and EIC data and may serve to reveal multi-parton correlation effects in QCD hard processes.

### 2.2.5 Unifying the Mechanisms for the Sivers effect

Recent developments have shown that the TMD approach and the collinear factorization approach can be unified to describe the Sivers effect for the single transverse-spin asymmetries in semi-inclusive DIS. The TMD approach covers the kinematic region $P_{h T} \ll Q$ where $Q \gg \Lambda_{\mathrm{QCD}}$, while the twist-3 approach covers the large $P_{h T}$ region, $P_{h T} \gg \Lambda_{\mathrm{QCD}}$. A natural question here is whether the two mechanisms give rise to equivalent (or consistent) SSA in the overlapping region, $\Lambda_{\mathrm{QCD}} \ll P_{h T} \ll Q$. To address this issue, we first recall the relation between the Sivers function $f_{1 T}^{\perp}\left(x, k_{\perp}\right)$ and the quark-gluon correlation function $G_{F}(x, x)$ [364: $\int d \boldsymbol{k}_{\perp}^{2} \boldsymbol{k}_{\perp}^{2} f_{1 T}^{\perp}\left(x, k_{\perp}\right)=\pi M_{N}^{2} G_{F}(x, x)$, which indicates that the two mechanisms are closely related.

A more explicit relation for the SSA in the two approaches has also been derived for the Sivers cross section, $F^{\sin \left(\phi_{h}-\phi_{S}\right)}$ in (2.27) 292, 294, 295): In the TMD approach, $F^{\sin \left(\phi_{h}-\phi_{S}\right)}$ is expressed in terms of the Sivers function $f_{1 T}^{\perp}\left(x, k_{\perp}\right)$. In the large $k_{\perp}$-region, relevant to $\Lambda_{\mathrm{QCD}} \ll P_{h T} \ll Q$, the $k_{\perp}$-dependence of $f_{1 T}^{\perp}\left(x, k_{\perp}\right)$ can be generated perturbatively, such that $f_{1 T}^{\perp}\left(x, k_{\perp}\right)$ is expressed as the convolution of the corresponding perturbative coefficient functions with the nonperturbative correlation functions $G_{F}$ and $\widetilde{G}_{F}$. By inserting this form of $f_{1 T}^{\perp}\left(x, k_{\perp}\right)$ into the TMD factorization formula for $F^{\sin \left(\phi_{h}-\phi_{S}\right)}$, one obtains the cross section written in terms of $G_{F}$ and $\widetilde{G}_{F}$, and this expression turns out to be identical to the leading $P_{h T}$ behavior of the twist-3 mechanism for $F^{\sin \left(\phi_{h}-\phi_{S}\right)}$ in the overlap region $\Lambda_{\mathrm{QCD}} \ll P_{h T} \ll Q$. From these studies, the two mechanisms for single-spin asymmetries represent a unique QCD effect over the entire $P_{h T}$ region. The same equivalence was also shown for the SSA in the Drell-Yan process. It should be noted that the sign of the Sivers function changes from SIDIS to the Drell-Yan case, while the twist-3 quark-gluon correlation functions are process-independent. The connection between the two mechanisms is also consistent with such process-(in)dependence [293].

The contribution from the twist-3 fragmentation function in (2.26) gives rise to the structure function $F^{\sin \left(\phi_{h}+\phi_{S}\right)}$ in (2.27), and dominates the leading $P_{h T}$ behavior of $F^{\sin \left(\phi_{h}+\phi_{S}\right)}$ compared to that from the quark-gluon correlation functions. This leading $P_{h T}$ behavior in $F^{\sin \left(\phi_{h}+\phi_{S}\right)}$ turns out to be identical to the corresponding contribution from the Collins function in the TMD approach, similarly as the above equivalence for $F^{\sin \left(\phi_{h}-\phi_{S}\right)}$ [297].

These are nontrivial and important results, which demonstrate that we indeed have a unique picture for single transverse-spin asymmetries in DIS and hadronic collisions. The discussion can be further generalized to other structure functions in SIDIS as well.

To analyze the general power behavior of the structure functions, it is important to realize that the power expansions are done in two different ways in the above two descriptions. At low $q_{T}$, first we expand in $\left(q_{T} / Q\right)^{n-2}$ and neglect terms with $n$ bigger than a certain value (so far, analyses have been carried out only up to $n=3$, i.e., twist- 3 ). To study the behavior at intermediate $q_{T}$ we further expand in $\left(M / q_{T}\right)^{k}$. Vice versa, at high $q_{T}$ we first expand in $\left(M / q_{T}\right)^{n}$ (also in this case, analyses are available up to $n=3$, i.e., twist-3). To study the intermediate- $q_{T}$ region, we further expand in $\left(q_{T} / Q\right)^{k-2}$. We can encounter two different situations:

- Type-I observables, where the leading terms at high and low transverse momentum have the same behavior. For instance,

$$
\begin{equation*}
F\left(q_{T}, Q\right)=A\left[\frac{q_{T}}{Q}\right]^{0}\left[\frac{M}{q_{T}}\right]^{2}+B\left[\frac{q_{T}}{Q}\right]^{2}\left[\frac{M}{q_{T}}\right]^{2}+\ldots \tag{2.28}
\end{equation*}
$$

where the term $A$ is leading in both the low- and high- $q_{T}$ calculations. In this case, the calculations at high and low transverse momentum must yield exactly the same result at intermediate transverse momentum [273, 292. If a mismatch occurs, it means that one of the calculations is incorrect or incomplete.

- Type-II observables, where the leading terms at high and low transverse momentum have different behavior. For instance,

$$
\begin{equation*}
F\left(q_{T}, Q\right)=A^{\prime}\left[\frac{q_{T}}{Q}\right]^{0}\left[\frac{M}{q_{T}}\right]^{4}+B^{\prime}\left[\frac{q_{T}}{Q}\right]^{2}\left[\frac{M}{q_{T}}\right]^{2}+\ldots \tag{2.29}
\end{equation*}
$$

where the first term is leading and the second term sub-leading in the low- $q_{T}$ calculation, whereas the reverse holds in the high- $q_{T}$ calculation. In this case, if the calculations at high and low transverse momentum are performed at their respective leading order, they describe two different mechanisms and will not lead to the same result at intermediate transverse momentum. In order to "match", the calculations should be carried out in both regimes up to the sub-subleading order. We could call this situation an "expected mismatch", since it is simply due to the difference between the two expansions.

In Tab. 2.3 we list the power behavior of the structure functions at intermediate transverse momentum, as obtained from the limits of the low- $q_{T}$ and high $-q_{T}$ calculation. For details of the calculation, we refer to [296]. The structure functions with a "yes" or "no" in the last column of Tab. 2.3 are type-I observables, where on the basis of power counting we know that two calculations describe the same physics and should therefore exactly match. In these cases, the high $q_{T}$ calculation describes the perturbative tail of the low- $q_{T}$ effect. The two mechanisms need not be distinguished. Using resummation it should be possible to construct expressions for these observables that are valid at any $q_{T}$. Six of these structure functions have been calculated explicitly.

For the functions identified as type-II in the last column of Tab. 2.3, the low $-q_{T}$ and high- $q_{T}$ calculations at leading order pick up two different components of the full structure function. They therefore describe two different mechanisms and do not match. For such type-II observables, if one aims at studying the leading-twist contribution from transverse momentum distributions, some considerations have to be kept in mind:

- the leading contribution from the high- $q_{T}$ calculation (often referred to as a pQCD or radiative correction) is a competing effect that has to be taken into account 365, 366, 367];
- $q_{T}$-weighted asymmetries enhance the high- $q_{T}$ mechanism and thus are not appropriate to extract type-II TMDs;
- it is at present impossible to construct an expression that extends the high- $q_{T}$ calculation to $q_{T} \approx M$, since this requires a smooth merging into unknown twist- 4 contributions, which most probably cannot be factorized (see also Ref. [368]);

| structure function | low- $q_{T}$ <br> power | high- $q_{T}$ <br> power | exact <br> match | structure <br> function | low- $q_{T}$ <br> power | high- $q_{T}$ <br> power | exact <br> match |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $F_{U U, T}$ | $1 / q_{T}^{2}$ | $1 / q_{T}^{2}$ | yes | $F_{U T, T}^{\sin \left(\phi_{h}-\phi_{S}\right)}$ | $1 / q_{T}^{3}$ | $1 / q_{T}^{3}$ | yes |
| $F_{U U}^{\cos 2 \phi_{h}}$ | $1 / q_{T}^{4}$ | $1 / Q^{2}$ | type II | $F_{U T}^{\sin \left(\phi_{h}+\phi_{S}\right)}$ | $1 / q_{T}^{3}$ | $1 / q_{T}^{3}$ | yes |
| $F_{U L}^{\sin 2 \phi_{h}}$ | $1 / q_{T}^{4}$ |  | (type II) | $F_{U T}^{\sin \left(3 \phi_{h}-\phi_{S}\right)}$ | $1 / q_{T}^{3}$ | $1 /\left(Q^{2} q_{T}\right)$ | type II |
| $F_{L L}$ | $1 / q_{T}^{2}$ | $1 / q_{T}^{2}$ | yes | $F_{L T}^{\cos \left(\phi_{h}-\phi_{S}\right)}$ | $1 / q_{T}^{3}$ |  | (yes) |

Table 2.3. Behavior of SIDIS structure functions in the region $M \ll q_{T} \ll Q$, as deduced from the low- $q_{T}$ calculation based on TMD factorization and the high- $q_{T}$ calculation based on collinear factorization. Empty fields indicate that no calculation is available. The last column indicates whether the expressions match exactly, do not match exactly, or should not be expected to match. In parentheses: expected answers based on analogy, rather than actual calculation.

- it is desirable from the experimental point of view to build observables that are least sensitive to the effect of radiative corrections.

We stress that the above considerations apply not only to semi-inclusive DIS, but also to Drell-Yan and $e^{+} e^{-}$annihilation [369], which have been already used to extract the BoerMulders and Collins functions [367, 370.

In summary, at the moment there is the hope to build descriptions of the structure functions that go from low to high transverse momentum for the five structure functions with a "yes" in the last column of Tab. 2.3.

### 2.2.6 From low to high transverse momentum

Based on the above results, we can write down a unique formula for the transverse momentum dependence. Following the procedure of [273], the differential cross section for the spin dependent SIDIS process can be written as,

$$
\begin{equation*}
\frac{d \Delta \sigma\left(S_{\perp}\right)}{d y d x_{B} d z_{h} d^{2} P_{h T}}=\frac{d \Delta \sigma^{\mathrm{TMD}}}{d y d x_{B} d z_{h} d^{2} P_{h T}}+\left(\frac{d \Delta \sigma^{\mathrm{CO}}}{d y d x_{B} d z_{h} d^{2} P_{h T}}-\left.\frac{d \Delta \sigma^{\mathrm{CO}}}{d y d x_{B} d z_{h} d^{2} P_{h T}}\right|_{P_{h T} \ll Q}\right) \tag{2.30}
\end{equation*}
$$

which is valid in the whole transverse momentum region at leading power of $1 / Q^{2}$. In the above equation, the first term comes from the TMD factorization formalism, and the second term from the collinear factorization, CO, with the twist-three quark-gluon correlations contributions. The second term will dominate the SSA at large transverse momentum, and its $q_{T}$-dependence can be calculated from perturbative QCD. On the other hand, at low transverse momentum $P_{h T} \ll Q$, the second term vanishes, because the two contributions are exactly the same in this limit, and cancel each other out. Experimentally, if we can study the transverse momentum dependence of the SSA for a wide range, we shall explore the transition from the perturbative region to the nonperturbative region.

The potential of the EIC for a study of this transition is illustrated in fig. [2.15, which shows the projected accuracy for single $\pi^{+}$production for a four-dimensional binning in the kinematic variables $x, Q^{2}, z$ and $P_{h T}$, using three different energy configurations for the EIC $(\sqrt{s}=15,50$ and 140 GeV$)$ and an integrated luminosity of $120 \mathrm{fb}^{-1}$ for each configuration. Events are selected for $0.05<y<0.9$ and $W^{2}>5 \mathrm{GeV}^{2}$ and for the $z$ range of $0.30<z<0.35$, as example. An overall detection efficiency of $50 \%$ and a beam polarization of $70 \%$ are assumed. The position of each point is according to its $x$ and $Q^{2}$


Figure 2.15. Four-dimensional representation of the projected accuracy for single $\pi^{+}$production in semi-inclusive DIS off the proton focussing on the transition region from low to high $P_{h T}\left(q_{T} \approx\right.$ $\left.P_{h T} / z_{h}\right)$ as indicated in the panels. The position of each point is according to its $Q^{2}$ and $x$ value for a specific bin in $z$ of $0.30<z<0.35$ and within the range $0.05<y<0.9$. The projected event rate, represented by the error bar, is scaled to the (arbitrarily chosen) asymmetry value at the right axis. Blue squares, black triangles and red dots represent the $\sqrt{s}=140 \mathrm{GeV}, \sqrt{s}=50 \mathrm{GeV}$ and $\sqrt{s}=15$ GeV EIC configurations, respectively. Event counts correspond to an integrated luminosity of 120 $\mathrm{fb}^{-1}$ for each of the three configurations.
value (abscissa and left ordinate, respectively) and each panel is for a $P_{h T}$ bin as indicated in the figure. The projected event rate is represented by the error bar scaled with respect to the (arbitrarily chosen) asymmetry value given at the right ordinate. The parameterization of Ref. [371] was used to simulate the cross section in the transition region. The simulation demonstrates that the transition region $q_{T} \approx P_{h T} / z_{h} \sim 4 \div 8 \mathrm{GeV}$ can be explored in great detail. Energies up to $\sqrt{s}=200 \mathrm{GeV}$ and longer running times will allow for exploring even higher values of $P_{h T}$.

The most important example to study the transition between low and high transverse momentum and the role of resummation is the structure function $F_{U U, T}$. The doublelongitudinal structure function $F_{L L}$ is the only other example where the theoretical framework has been developed at the same level [372].

Fig. 2.16 shows an example of resummation results for DIS at a high-energy EIC option. These results give us an idea of the extension of the region of intermediate transverse momentum (and therefore also of the regions of high and low transverse momentum). This extension obviously depends on experimental kinematics, in particular on $Q^{2}$. As a lower boundary of this region we can consider the values of $q_{T}$ where the nonperturbative component of the Sudakov factor becomes relevant. As an upper boundary we can consider the values of $q_{T}$ for which the fixed-order cross section becomes comparable to the resummed cross section. From fig. 2.16 we can estimate that the intermediate-transverse-momentum region corresponds to $4 \mathrm{GeV} \lesssim q_{T} \lesssim 8 \mathrm{GeV}$.

A lot remains to be done to better pin down the nonperturbative Sudakov factors, their functional form, their flavor dependence, and their errors. This should be a high-priority


Figure 2.16. Unpolarized SIDIS cross section for EIC kinematics from Ref. [372]. Shown are: the fixed-order result, the resummation results with different high- $b$ regularizations and different values of the nonperturbative Sudakov factor.
task for the EIC. The same is true for the doubly-longitudinally polarized case, where the nonperturbative components are unknown.

To conclude this section, we mention that the same program of resumming radiative contributions should be pursued also for the Sivers, Collins, and $F_{L T}^{\cos \left(\phi_{h}-\phi_{S}\right)}$ structure functions. At the moment the only discussion of similar topics is done in sec. 9 of Ref. [369]. However, we can expect developments in this direction in the near future and hope to obtain an expression of the above-mentioned structure functions that includes transverse-momentum resummation and describes the physics in the whole transverse-momentum spectrum.

### 2.2.7 Weighted Asymmetries

Currently, experimental studies in semi-inclusive DIS have limited access to single-spin asymmetries at large transverse momentum, and most of the data are in the low transverse momentum region, where the TMD formalism dominates. In phenomenological studies, in order to compare with the experimental data, one has to make model assumptions for the transverse momentum dependence of the distribution and fragmentation functions. However, there is a class of observables that does not require detailed model assumptions about transverse momentum dependence. These are transverse momentum weighted single-spin asymmetries, which transform the convolutions in the factorized cross section into simple products [244, 373].

Staying for the moment in the framework of collinear factorization, an example for a weighted differential cross section at leading order in $\alpha_{s}$ is

$$
\begin{equation*}
\int d^{2} P_{h T} \frac{P_{h T}}{z_{h} M_{P}} \sin \left(\phi_{h}-\phi_{S}\right) \frac{d \Delta \sigma^{\mathrm{TMD}}\left(S_{\perp}\right)}{d x_{B} d y d z_{h} d^{2} \vec{P}_{h T}}=\sigma_{0} \sum_{q} e_{q}^{2} \frac{g_{s}}{2 M_{P}} T_{F}^{q}(x) D(z) \tag{2.31}
\end{equation*}
$$

where $e_{q}$ is the electric charge for a quark of flavor $q$, and where $T_{F}(x)$ is the Qiu-Sterman matrix element of the quark-gluon correlation function, and has been defined above. With the standard choice of $P_{h T}$-weights $w_{1}=P_{h T} / z_{h} M_{P}$ for the numerator and $w_{0}=1$ for the
denominator, the $P_{h T}$-weighted Sivers-asymmetry thus becomes

$$
\begin{equation*}
\frac{\left\langle\frac{P_{h T}}{z_{h} M_{P}} \sin \left(\phi_{h}-\phi_{S}\right)\right\rangle_{\mathrm{UT}}}{\langle 1\rangle_{\mathrm{UU}}}=\frac{\frac{1}{Q^{4}}\left(1-y+\frac{y^{2}}{2}\right) \frac{x_{B}}{2 M_{P}} \sum_{q} e_{q}^{2} g_{s} T_{F}^{q}(x) D(z)}{\frac{1}{Q^{4}}\left(1-y+\frac{y^{2}}{2}\right) x_{B} \sum_{q} e_{q}^{2} f_{1}(x) D(z)} . \tag{2.32}
\end{equation*}
$$

We can go beyond the above leading order results and establish a collinear factorization formalism for the weighted single transverse spin dependent cross section. A similar study has been performed for the Drell-Yan lepton pair production process, where a next-to-leading order perturbative corrections have been obtained [291]. We expect similar calculations for SIDIS shall appear soon.

Recently, a generalization to employ Bessel functions as weights $w_{n} \propto J_{n}\left(\left|\mathbf{P}_{h T}\right| \mathcal{B}_{T}\right)$ has been suggested [374. The Sivers asymmetry with generalized weights reads

$$
\begin{align*}
& \frac{\left\langle\frac{2 J_{1}\left(\left|\mathbf{P}_{h T}\right| \mathcal{B}_{T}\right)}{z M \mathcal{B}_{T}} \sin \left(\phi_{h}-\phi_{s}\right)\right\rangle_{U T}}{\left\langle J_{0}\left(P_{h T} \mathcal{B}_{T}\right)\right\rangle}= \\
& \quad-2 \frac{\frac{1}{Q^{4}}\left(1-y+\frac{y^{2}}{2}\right) \sum_{q} e_{q}^{2} \tilde{f}_{1 T}^{\perp(1) q}\left(x, z^{2} \mathcal{B}_{T}^{2}\right) \tilde{D}\left(z, \mathcal{B}_{T}^{2}\right)}{\frac{1}{Q^{4}}\left(1-y+\frac{y^{2}}{2}\right) \sum_{q} e_{q}^{2} \tilde{f}_{1}\left(x, z^{2} \mathcal{B}_{T}^{2}\right) \tilde{D}_{1}\left(z, \mathcal{B}_{T}^{2}\right)}, \tag{2.33}
\end{align*}
$$

where now $\tilde{f}_{1 T}^{\perp(1) q}, \tilde{f}_{1}^{q}$ and $\tilde{D}$ are TMDs and TMD FFs Fourier transformed with respect to transverse momentum. In the asymptotic limit $\mathcal{B}_{T} \rightarrow 0$, we recover the conventional weighted asymmetry Eq. (2.32), and the Fourier transformed TMDs and FFs can be identified with the moments in that equation.

An important advantage of the generalized weights is that a non-zero choice of the parameter $\mathcal{B}_{T}$ can reduce the sensitivity to large transverse momenta. This property also applies to the Fourier transformed TMDs and TMD FFs entering the asymmetries. The new approach thus avoids the problem of divergent $k_{\perp}$-integrals that affects moments of TMDs and TMD FFs. Additionally, the analysis in Ref. 374 shows that soft factors appearing beyond tree level cancel out of the weighted asymmetry.

We conclude that an EIC presents a unique opportunity to obtain the necessary coverage and resolution in $P_{h T}$ to explore the nucleon spin structure in the language of weighted asymmetries.

### 2.3 Transverse polarization effects with gluons

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The gluon Sivers function shares the same characteristic features as its counterpart in the quark sector, the quark Sivers function, as discussed in the last section. Among the important information we can obtain from this distribution is the spin-orbit correlation of gluons inside the nucleon, which will help us to understand the gluon spin contribution to the proton spin. The EIC is the unique machine to map out in much detail the gluon distribution, including the spin-dependent and spin-averaged transverse momentum dependent distributions. In this section, we will focus on the gluon Sivers function. The study of this distribution is strongly related to other measurements such as the gluon GPDs and the unintegrated gluon distributions of nucleon/nucleus at small- $x$.

Various processes in DIS can be used to probe the transverse momentum dependent gluon distributions, such as heavy quark and quarkonium production. Also the dijet/dihadron correlation has been proposed as a promising probe for the gluon Sivers function and other TMD gluon distributions.

In Ref. [375], it was suggested to use the dijet-correlation to study the gluon Sivers function in $p p$ collisions. However, because of both initial and final state interaction effects involved in $p p$ scattering, the factorization of this process is shown to be broken (see detailed discussions in next section). On the other hand, for the DIS processes, because only one hadron is involved in the initial state, the dijet-correlation process could be factorized in the same spirit as the semi-inclusive hadron production discussed in the previous sections.

We consider here the dijet/quark-antiquark production in DIS

$$
\begin{equation*}
\gamma^{*} N^{\uparrow} \rightarrow H_{1}\left(k_{1}\right)+H_{2}\left(k_{2}\right)+X, \tag{2.34}
\end{equation*}
$$

where $N$ represents the transversely polarized nucleon, $H_{1}$ and $H_{2}$ are the two final state particles with momenta $k_{1}$ and $k_{2}$, respectively. We are interested in the kinematic region where the transverse momentum imbalance between them is much smaller than the individual transverse momenta: $k_{\perp}=\left|\boldsymbol{k}_{1 T}+\boldsymbol{k}_{2 T}\right| \ll P_{J T}$ where $\boldsymbol{P}_{J T}$ is defined as $\left(\boldsymbol{k}_{1 T}-\boldsymbol{k}_{2 T}\right) / 2$. This is referred to as the (back-to-back) correlation limit. An important advantage of taking this correlation limit is that we can apply the power counting method to obtain the leading order contribution of $k_{\perp} / P_{J T}$ where the differential cross section directly depends on the TMD gluon distribution. As illustrated in Fig. [2.17, with transverse spin in the dijet plane, the correlation between the two jets will lead to a preferred direction in the transverse plane. This will signal the gluon Sivers effect if the process is dominated by the gluonic subprocesses.

As demonstrated in Ref. [283], the TMD gluon distribution in the quark-antiquark jet correlation in the DIS process of (2.34) follows the original gluon distribution definition of Ref. [241],

$$
\begin{equation*}
x f_{1}^{g}\left(x, k_{\perp}\right)=\int \frac{d \xi^{-} d^{2} \xi_{\perp}}{(2 \pi)^{3} P^{+}} e^{i x P^{+} \xi^{-}-i k_{\perp} \cdot \xi_{\perp}}\langle P| F^{+i}\left(\xi^{-}, \xi_{\perp}\right) \mathcal{L}_{\xi}^{\dagger} \mathcal{L}_{0} F^{+i}(0)|P\rangle \tag{2.35}
\end{equation*}
$$

where $F^{\mu \nu}$ is the gauge field strength tensor $F_{a}^{\mu \nu}=\partial^{\mu} A_{a}^{\nu}-\partial^{\nu} A_{a}^{\mu}-g f_{a b c} A_{b}^{\mu} A_{c}^{\nu}$ with $f_{a b c}$ the antisymmetric structure constants for $S U(3)$, and the gauge-link follows the similar definition as that for the quark distribution but in the adjoint representation. The physics behind


Figure 2.17. Back-to-back dijet correlation can be used to probe the TMD gluon distributions.
this factorization is the following. The virtual photon scatters on the nucleon target and produces a quark-antiquark pair through the partonic process $\gamma^{*} g \rightarrow q \bar{q}$. In the correlation limit, the quark-antiquark pair stays close in the coordinate space, and act as a color-octet object, which effectively behaves like a single gluon. In particular, the net effect of the final state interactions between the nucleon target and the quark-antiquark pair is exactly the same antisymmetric structure $f_{a b c}$ as in the TMD gluon definition of Eq. (2.35). This is totally different from the analogous QED process where the final state interactions cancel out completely with the fermion-antifermion pair.

In the following, we will present some recent phenomenological studies on the gluon TMDs from the quark-antiquark correlation in DIS processes. We expect more interesting results shall be obtained in the near future.

### 2.3.1 The gluonic Sivers effect in dihadron production

The production of a pair of hadrons with high transverse momenta in DIS is sensitive to the transverse-momentum dependent gluon distribution. In particular, it has a transverse target spin asymmetry due to the gluon Sivers function. The relevant parton-level subprocess is $\gamma^{*} g \rightarrow q \bar{q}$, and to eliminate contributions from $\gamma^{*} q \rightarrow q g$ and $\gamma^{*} \bar{q} \rightarrow \bar{q} g$ we focus on charm production.

As a straight forward generalization of the unpolarized case recently studied in 283], the cross section for the dijet/c $\bar{c}$ production from a nucleon with transverse polarization $S_{\perp}$ can be written as

$$
\begin{equation*}
\frac{d \sigma^{\gamma_{T, L}^{*} p \rightarrow c \bar{c}+X}}{d z d^{2} k_{1 T} d^{2} k_{2 T}}=\frac{H^{\gamma_{T, L}^{*} g \rightarrow c \bar{c}}}{z \bar{z}}\left[f_{1}^{g}\left(x, k_{\perp}\right)+\frac{\left(\boldsymbol{S}_{\perp} \times \boldsymbol{k}_{\perp}\right)^{3}}{M} f_{1 T}^{g \perp}\left(x, k_{\perp}\right)\right] . \tag{2.36}
\end{equation*}
$$

Here, $f_{1}^{g}$ is the usual gluon TMD, $f_{1 T}^{g \perp}$ the gluon Sivers distribution and $\bar{z}=1-z$. Again, we are interested in the back-to-back correlation limit. The gluon momentum fraction is then given by $x / x_{B} \approx 1+\left(P_{J T}^{2}+m_{c}^{2}\right) /\left(z \bar{z} Q^{2}\right)$, where $m_{c}$ is the charm quark mass. The hard-scattering cross sections $H^{\gamma_{T, L}^{*} g \rightarrow c \bar{c}}$ for transverse and longitudinal photons depend on $P_{h T}^{2}, Q^{2}, z$ and $m_{c}$ and can be found in [283].

It may be possible to study the cross section (2.36) experimentally through the production of two heavy-quark jets, but the interpretation of this process requires a quantitative
understanding of the relative transverse momentum between a reconstructed jet and the heavy quark it originates from. As an alternative, we consider here the production of two heavy hadrons, e.g. $D$ mesons. Its cross section reads

$$
\begin{align*}
& \frac{d \sigma_{T, L}^{*} p \rightarrow h_{1} h_{2}+X}{d z_{1} d z_{2} d^{2} P_{h_{1} T} d^{2} P_{h_{2} T}}=\int_{z_{1}}^{1-z_{2}} d z \frac{H^{\gamma_{T, L}^{*} g \rightarrow c \bar{c}}}{z^{2} \bar{z}^{2}} \int d^{2} \lambda_{1 T} d^{2} \lambda_{2 T}\left[f_{1}^{g}\left(x, k_{\perp}\right)\right. \\
& \left.\quad+\frac{\left(\boldsymbol{S}_{\perp} \times \boldsymbol{k}_{\perp}\right)^{3}}{M} f_{1 T}^{g \perp}\left(x, k_{\perp}\right)\right] D^{h_{1} / c}\left(\frac{z_{1}}{z}, \frac{z_{1}}{z} \lambda_{1 T}\right) D^{h_{2} / \bar{c}}\left(\frac{z_{2}}{\bar{z}}, \frac{z_{2}}{\bar{z}} \lambda_{2 T}\right) \tag{2.37}
\end{align*}
$$

where

$$
\begin{equation*}
\boldsymbol{k}_{1 T}=\boldsymbol{\lambda}_{1 T}+\frac{z}{z_{1}} \boldsymbol{P}_{h_{1} T}, \quad \quad \boldsymbol{k}_{2 T}=\boldsymbol{\lambda}_{2 T}+\frac{\bar{z}}{z_{2}} \boldsymbol{P}_{h_{2} T} . \tag{2.38}
\end{equation*}
$$

Here $h_{1}$ is the hadron containing a $c$ quark and $h_{2}$ the one containing a $\bar{c}$, with $\boldsymbol{P}_{h_{1} T}, \boldsymbol{P}_{h_{2} T}$ denoting their transverse momenta and $z_{1}, z_{2}$ their momentum fractions w.r.t. the virtual photon. The fragmentation functions $D\left(z, P_{\perp}\right)$ depend on the momentum fraction $z$ and the relative transverse momentum $P_{\perp}$ of the hadron with respect to the quark or antiquark.

The parton-level variables $\boldsymbol{k}_{1 T}, \boldsymbol{k}_{2 T}$ and $z$ are not directly measurable, but a detailed analysis of the kinematics [376] reveals that they can be partly determined from the hadronic final state. In particular, one can define variables $\boldsymbol{k}_{\perp}^{\prime}, \boldsymbol{P}_{T}^{\prime}$ and $z^{\prime}$ that are measurable and closely related to $\boldsymbol{k}_{\perp}=\boldsymbol{k}_{1 T}+\boldsymbol{k}_{2 T}, \boldsymbol{P}_{T}=\left(\boldsymbol{k}_{1 T}-\boldsymbol{k}_{2 T}\right) / 2$ and $z$, respectively. The cross product ( $\boldsymbol{S}_{\perp} \times \boldsymbol{k}_{\perp}$ ) in (2.37) gives rise to an angular modulation

$$
\begin{equation*}
\frac{d \sigma^{\gamma^{*} p \rightarrow h_{1} h_{2}+X}}{d k^{\prime} d \phi_{S, k^{\prime}}} \approx A\left(k_{\perp}^{\prime}\right)+B\left(k_{\perp}^{\prime}\right) \sin \left(\phi_{S k^{\prime}}+\gamma\right), \tag{2.39}
\end{equation*}
$$

where $\phi_{S k^{\prime}}$ is the azimuthal angle between $\boldsymbol{S}_{\perp}$ and $\boldsymbol{k}_{\perp}^{\prime}$. The coefficient $B\left(k^{\prime}\right)$ depends on the gluon Sivers function, as well as the phase $\gamma$.

To estimate the possible size of the Sivers asymmetry, we follow [377] and assume

$$
\begin{equation*}
f_{1 T}^{g \perp}\left(x, k_{\perp}\right)=\frac{2 \sigma M}{k_{\perp}^{2}+\sigma^{2}} f_{1}^{g}\left(x, k_{\perp}\right), \quad \quad f_{1}^{g}\left(x, k_{\perp}\right)=\frac{e^{-k_{\perp}^{2} / \sigma^{2}}}{\pi \sigma^{2}} f_{1}^{g}(x) \tag{2.40}
\end{equation*}
$$

with $\sigma=800 \mathrm{MeV}$ and the integrated gluon distribution $f_{1}^{g}(x)$ from MSTW 2008 [22]. This Ansatz saturates the positivity bound $\frac{k_{\perp}}{M}\left|f_{1 T}^{g \perp}\left(x, k_{\perp}\right)\right| \leq f_{1}^{g}\left(x, k_{\perp}\right)$ at $k_{\perp}=\sigma$ and undershoots it for all other values of $k_{\perp}$. We consider the production of $D$ meson pairs and take a fragmentation function $D\left(z, P_{\perp}\right)=D(z) e^{-P_{\perp}^{2} / \sigma^{2}} /\left(\pi \sigma^{2}\right)$ with the same Gaussian width as in (2.40). We take $D(z) \propto z^{\alpha}(1-z)^{\beta} e^{\gamma z(1-z)}$ with $\alpha=2.86, \beta=1.57, \gamma=5.66$, which gives a fair description of the $D^{0}$ spectrum observed in $e^{+} e^{-}$annihilation [221, 220]. In Fig. 2.18 we show the transverse target spin asymmetry

$$
\begin{equation*}
A\left(k_{\perp}^{\prime}, \phi_{S k^{\prime}}\right)=\frac{d \sigma\left(k_{\perp}^{\prime}, \phi_{S k^{\prime}}\right)-d \sigma\left(k_{\perp}^{\prime}, \phi_{S k^{\prime}}+\pi\right)}{d \sigma\left(k_{\perp}^{\prime}, \phi_{S k^{\prime}}\right)+d \sigma\left(k_{\perp}^{\prime}, \phi_{S k^{\prime}}+\pi\right)} \tag{2.41}
\end{equation*}
$$

for the process $\gamma^{*} p \rightarrow D^{0} \bar{D}^{0}+X$ summed over transverse and longitudinal photon polarization. We find that the phase shift $\gamma$ in (2.39) is tiny. The asymmetry is found to be sizable with our Ansatz, which suggests that DIS production of heavy meson pairs at EIC has good sensitivity to the gluon Sivers function.


Figure 2.18. The transverse target asymmetry (2.41) for $\gamma^{*} p \rightarrow D^{0} \bar{D}^{0}+X$. The kinematics is specified by $W=100 \mathrm{GeV}, Q^{2}=16 \mathrm{GeV}^{2}, z_{1}=z_{2}=0.3,0.25<z^{\prime}<0.75$ and $5 \mathrm{GeV}<P_{T}^{\prime}<$ 40 GeV .

### 2.3.2 Probing the linear polarization of gluons in unpolarized hadrons

Gluons inside unpolarized hadrons can be linearly polarized provided they have a nonzero transverse momentum. The simplest and theoretically safest way to probe this TMD distribution of linearly polarized gluons is through $\cos 2 \phi$ asymmetries in heavy quark pair or dijet production in electron-hadron collisions. Future EIC or LHeC experiments are ideally suited for this purpose. Here we estimate the maximum asymmetries for EIC kinematics.

Linearly polarized gluons in an unpolarized hadron, carrying a light-cone momentum fraction $x$ and transverse momentum $\boldsymbol{k}_{\perp}$ w.r.t. to the parent's momentum, are described by the TMD $h_{1}^{\perp g}\left(x, k_{\perp}\right)$ [281, 284, 378. Unlike the quark TMD $h_{1}^{\perp q}$ of transversely polarized quarks inside an unpolarized hadron (also frequently referred to as Boer-Mulders function) [244], $h_{1}^{\perp g}$ is chiral-even and $T$-even. This means it does not require initial or final state interactions (ISI/FSI) to be non-zero. Nevertheless, as any TMD, $h_{1}^{\perp g}$ can receive contributions from ISI or FSI and therefore can be process dependent, in other words, non-universal, and its extraction can be hampered in non-factorizing cases.

Thus far no experimental studies of $h_{1}^{\perp g}$ have been performed. As recently pointed out, it is possible to obtain an extraction of $h_{1}^{\perp g}$ in a simple and theoretically safe manner, since unlike $h_{1}^{\perp q}$ it does not need to appear in pairs [284. Here we will discuss observables that involve only a single $h_{1}^{\perp g}$ in semi-inclusive DIS to two heavy quarks or to two jets, which allow for TMD factorization and hence a safe extraction. The corresponding hadroproduction processes run into the problem of factorization breaking [272, 284].

Again, we consider heavy quark production, $e(\ell)+h(P) \rightarrow e\left(\ell^{\prime}\right)+Q\left(k_{1}\right)+\bar{Q}\left(k_{2}\right)+X$, where the four-momenta of the particles are given within brackets, and the heavy quark-antiquark pair in the final state is almost back-to-back in the plane perpendicular to the direction of the exchanged photon and hadron. The calculation proceeds along the lines explained in Refs. [378, 379]. We obtain for the cross section integrated over the angular distribution of


Figure 2.19. Upper bounds of the asymmetry ratio $R$ in equation (2.44) as a function of $\left|\boldsymbol{P}_{J T}\right|$ at different values of $Q^{2}$, with $y=0.01$ and $z=0.5$.
the back-scattered electron $e\left(\ell^{\prime}\right)$ :

$$
\begin{equation*}
\frac{d \sigma}{d y_{1} d y_{2} d y d x_{B} d^{2} \boldsymbol{k}_{\perp} d^{2} \boldsymbol{P}_{J T}}=\frac{\alpha^{2} \alpha_{s}}{\pi s M_{T}^{2}} \frac{\left(1+y x_{B}\right)}{y^{5} x_{B}}\left(A+\frac{\boldsymbol{k}_{\perp}^{2}}{M^{2}} B \cos 2 \phi\right) \delta\left(1-z_{1}-z_{2}\right)( \tag{2.42}
\end{equation*}
$$

The kinematics are the same as in the last subsection with the heavy quark mass $M_{Q}$, $M_{i T}^{2} \approx M_{T}^{2}=M_{Q}^{2}+P_{J T}^{2}$ and the rapidities $y_{i}$ for the quark momenta along photon-target direction. The azimuthal angles of $\boldsymbol{k}_{\perp}$ and $\boldsymbol{P}_{J T}$ are denoted by $\phi_{\perp}$ and $\phi_{T}$, respectively, and $\phi \equiv \phi_{\perp}-\phi_{T}$. The functions $A$ and $B$ depend on $y, z\left(\equiv z_{2}\right), Q^{2} / M_{T}^{2}, M_{Q}^{2} / M_{T}^{2}$, and $\boldsymbol{k}_{\perp}^{2}$. The angular independent part $A$ involves only the unpolarized TMD gluon distribution $f_{1}^{g}$, while the magnitude $B$ of the $\cos 2 \phi$ asymmetry is determined by $h_{1}^{\perp g}\left(x, k_{\perp}\right)$. Since $h_{1}^{\perp g}$ is completely unknown, we estimate the maximum asymmetry that is allowed by the bound [284]

$$
\begin{equation*}
\left|h_{1}^{\perp g(2)}(x)\right| \leq \frac{\left\langle k_{\perp}^{2}\right\rangle}{2 M^{2}} f_{1}^{g}(x), \tag{2.43}
\end{equation*}
$$

where the superscript (2) denotes the $n=2$ transverse moment (defined as $f^{(n)}(x) \equiv$ $\left.\int d^{2} \boldsymbol{k}_{\perp}\left(\boldsymbol{k}_{\perp}^{2} / 2 M^{2}\right)^{n} f\left(x, \boldsymbol{k}_{\perp}^{2}\right)\right)$. The maximal (absolute) value of the asymmetry ratio

$$
\begin{equation*}
R=\left|\frac{\int d^{2} \boldsymbol{k}_{\perp} \boldsymbol{k}_{\perp}^{2} \cos 2\left(\phi_{\perp}-\phi_{T}\right) d \sigma}{\int d^{2} \boldsymbol{k}_{\perp} \boldsymbol{k}_{\perp}^{2} d \sigma}\right|=\frac{\int d \boldsymbol{k}_{\perp}^{2} \boldsymbol{k}_{\perp}^{4}|B|}{2 M^{2} \int d \boldsymbol{k}_{\perp}^{2} \boldsymbol{k}_{\perp}^{2} A} \tag{2.44}
\end{equation*}
$$

is depicted in Fig. 2.19 as a function of $\left|\boldsymbol{P}_{J T}\right|$ at different values of $Q^{2}$ for charm (left panel) and bottom (right panel) production, where we have selected $y=0.01, z=0.5$, and taken $M_{c}^{2}=2 \mathrm{GeV}^{2}, M_{b}^{2}=25 \mathrm{GeV}^{2}$. Such large asymmetries, together with the relative simplicity of the suggested measurement (polarized beams are not required), would probably allow an extraction of $h_{1}^{\perp g}\left(x, k_{\perp}\right)$ at the EIC (or LHeC).

### 2.4 Theory highlights

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The candidates for the golden measurement at the EIC are the spin-dependent Sivers function $f_{1 T}^{\perp}$, as well as the unpolarized quark distribution $f_{1}$. The proposed silver candidates are the transversity, the Boer-Mulders, and the Collins functions. All these objects are transverse-momentum dependent parton densities that describe the inner structure of hadrons by taking into account the longitudinal and the transversal partonic degrees of freedom.

In the last few years, there has been tremendous progress on the theory developments for the transverse momentum dependent parton distributions. In particular, there have been intensive investigations on the QCD factorization and the associated universality of the TMD parton distributions in various hard processes; the energy scale dependence for the TMD distributions and related quark-gluon correlation functions. In this section, we will highlight these developments.

### 2.4.1 Gauge-links, TMD-factorization, and TMD-factorization breaking

In this section, we discuss some basic features of transverse momentum dependent parton distribution functions. In hard processes, parton distribution functions and fragmentation functions are expressed as matrix elements of nonlocal combinations of quark or gluon fields. In the collinear situation that all transverse momenta of partons are integrated over in the definitions, the nonlocality is in essence light-like. These correlation functions are convoluted with the squared amplitude for the partonic subprocess (in essence the partonic cross section) of a hard process. When the transverse momenta of partons are involved, the non-locality in the matrix elements includes a transverse separation, and a transverse momentum dependent (TMD) factorization theorem is needed. In all cases the definitions of the non-perturbative functions include gluon contributions resummed into gauge-links (or Wilson lines) that bridge the nonlocality.

It is important to realize that the appearance of the gauge-links is a consequence of the systematic resummation of extra gluon contributions in the derivations of factorization, so their structure is dictated by the requirements of factorization.

In processes like $\ell+H \longrightarrow \ell^{\prime}+h+X$ (semi-inclusive DIS), $\ell+\bar{\ell} \longrightarrow h_{1}+h_{2}+X$ (annihilation process) or $H_{1}+H_{2} \longrightarrow \ell+\bar{\ell}+X$ (Drell-Yan process) one has, at leading power in the hard scale, a simple underlying hard process, which is a virtual photon (or weak boson) coupling to a parton line. The color flow from the hard part to collinear or soft parts is simple. Additional gluons with polarizations collinear to the parton momenta are resummed into gauge-links, which exhibit the interesting behavior that for transverse momentum dependent functions they bridge the transverse separation between the nonlocal field combinations at lightcone past or future infinity. Which gauge-link is relevant in a particular non-perturbative function depends on the color flow in the full process. For a quark distribution function one has a link via (future) lightcone $+\infty$ if the color flows into the final state, and a link via (past) lightcone $-\infty$ if the color is annihilated by another incoming parton.

QCD factorization theorems are central to understanding high energy hadronic scattering cross sections in terms of the fundamentals of perturbative QCD. In addition to
providing a practical prescription for order-by-order calculations, derivations of factorization provide a solid theoretical underpinning for concepts like PDFs and FFs which are crucial in the quest to expand the basic understanding of hadronic structure. The most natural first attempt at a TMD-factorization formula is simply to extend the classic parton model intuition familiar from collinear factorization. For the semi-inclusive deep inelastic scattering (SIDIS) cross section, for example, the cross section might be written schematically as

$$
\begin{equation*}
d \sigma \sim|\mathcal{H}|^{2} \otimes \Phi\left(x, \boldsymbol{k}_{\perp}\right) \otimes D\left(z, \boldsymbol{P}_{\perp}\right) \delta^{(2)}\left(\boldsymbol{q}_{T}+\boldsymbol{k}_{\perp}-\boldsymbol{P}_{\perp}\right) . \tag{2.45}
\end{equation*}
$$

Here $\Phi\left(x, \boldsymbol{k}_{\perp}\right)$ is the TMD PDF while $D\left(z, \boldsymbol{P}_{\perp}\right)$ is the TMD FF, with the usual probability interpretations, and $|\mathcal{H}|^{2}$ represents the hard part. The momentum $\boldsymbol{q}_{T}$ is the small momentum sensitive to intrinsic transverse momenta, $\boldsymbol{k}_{\perp}$ and $\boldsymbol{P}_{\perp}$, carried by the colliding proton and the produced hadron. The $\otimes$ symbol denotes all relevant convolution integrals, and the $x$ and $z$ arguments are the usual longitudinal momentum fractions.

In a perturbative derivation of factorization, a small-coupling perturbative expansion of the cross section is analyzed in terms of "leading regions", and the sum is shown order-by-order to separate into the factors of Eq. (2.45). The precise field theoretic definitions of the correlation functions, $\Phi\left(x, \boldsymbol{k}_{\perp}\right)$ and $D\left(z, \boldsymbol{P}_{\perp}\right)$, should emerge naturally from the requirements of factorization. In the hard part $|\mathcal{H}|^{2}$, all propagators must be off-shell by order the hard scale $Q$ so that asymptotic freedom applies, and small-coupling perturbation theory is valid, with non-factorizing higher-twist contributions suppressed by powers of $Q$. Such factorization theorems are well-established for inclusive processes that utilize the standard integrated correlation functions (see [380] and references therein), but TMDfactorization theorems involve other subtleties, particularly with regard to the definitions of the TMD PDFs and FFs and their associated gauge-links.

In cases where there is a more complex color flow such as is often the case when the underlying hard process involves multiple color flows and/or if the incoming partons are gluons, this can potentially lead to a more complex gauge-link structure including traced closed loops or looping gauge-links. For situations in which only one TMD correlation function is studied, these structures have been examined in [265, [267, 381, 382] for two-totwo partonic subprocesses. In situations that involve several TMD functions, factorization using separate TMD functions fails completely.

To understand the issues that arise in defining TMDs, it is instructive to start with a review of the definition of the standard integrated quark PDF. It is

$$
\begin{equation*}
f(x ; \mu)=\text { F.T. }\langle p| \bar{\psi}\left(0, w^{-}, \mathbf{0}_{t}\right) \gamma^{+} V_{[0, w]}\left(u_{\mathrm{J}}\right) \psi(0)|p\rangle, \tag{2.46}
\end{equation*}
$$

where "F.T." stands for the Fourier transform from coordinate space to momentum space. The above definition contains UV divergences which must be renormalized. This gives dependence on an extra scale $\mu$, and ultimately results in the well-known DGLAP evolution equations for the integrated PDF. For a gauge invariant definition, the PDF must contain a path ordered exponential of the gauge field that connects the points 0 and $\left(0, w^{-}, \mathbf{0}_{t}\right)$. This is the gauge-link and its formal definition is

$$
\begin{equation*}
V_{[0, w]}\left(u_{\mathrm{J}}\right)=P \exp \left(-i g t^{a} \int_{0}^{w^{-}} d \lambda u_{J} \cdot A^{a}\left(\lambda u_{J}\right)\right) . \tag{2.47}
\end{equation*}
$$

The path of the gauge-link is determined by the light-like vector $u_{\mathrm{J}}=\left(0,1, \mathbf{o}_{t}\right)$. That is, the gauge-link follows a straight path connecting 0 and $\left(0, w^{-}, \mathbf{0}_{t}\right)$ along the exactly


Figure 2.20. (a) Target-collinear gluons in a graph for SIDIS. (b) Factorization of extra gluons into gauge-link contributions.
light-like minus direction. In Feynman graph calculations, the contribution from the gaugelink corresponds to the so-called "eikonal factors," which have definite Feynman rules that follow naturally from factorization proofs. After a sum over graphs, and the application of appropriate approximations and Ward identity arguments, extra collinear gluons like those shown in Fig. [2.20(a) for SIDIS factor into gauge-link contributions. In Fig. 2.20(b), the eikonal factors are shown as gluon attachments from the target-collinear bubble to a double line.

The most natural first try at extending the PDF definition in Eq. (2.46) to the TMD case is to simply leave the integration over transverse momentum in the TMD PDF definition undone. That is, instead of Eq. (2.46) one may try

$$
\begin{equation*}
\Phi\left(x, \boldsymbol{k}_{t}\right)=\text { F.T. }\langle p| \bar{\psi}\left(0, w^{-}, \boldsymbol{w}_{t}\right) \gamma^{+} U_{[0, w]}\left(u_{J}\right) \psi(0)|p\rangle . \tag{2.48}
\end{equation*}
$$

The separation is now 0 and $\left(0, w^{-}, \boldsymbol{w}_{t}\right)$ - it has acquired a transverse component and the Fourier transform is now in both $w^{-}$and $\boldsymbol{w}_{t}$. As a result, the structure of the gauge-link $U_{[0, w]}\left(u_{J}\right)$ must also be modified from the simple straight light-like $V_{[0, w]}\left(u_{\mathrm{J}}\right)$ gauge-link of Eq. (2.46). The eikonal attachments on either side of the cut in Fig. 2.20 still give minusdirection Wilson lines, but now in order to have a closed link there must also be a small transverse detour at light-cone infinity. This detour arises naturally from boundary terms that are needed as subtractions to make higher twist contributions gauge invariant [263, 264].

The gauge-link structure in Eq. (2.48), with its two exactly light-like legs and a transverse link at infinity is commonly cited as the gauge-link that is necessary for the definition of the TMD PDFs. However, there are a number of further subtleties, and we will find that the definition needs to be modified. One complication is that rapidity divergences, which in collinear factorization would cancel in the sum of graphs, remain uncanceled in the definition of the TMD correlation functions. Rapidity divergences correspond to gluons moving with infinite rapidity in the direction opposite the containing hadron, and remain even when infrared gluon mass regulators are included. (For a more complete review of these and related issues, see for example [259, [383].) The most common way to regularize the lightcone divergences is to make the gauge links slightly non-light-like. In the coordinate space picture, the gauge-link therefore becomes more like the tilted hook shape. This introduces a new arbitrary rapidity parameter - the "tilt" of the gauge-link. A generalization of renormalization group techniques is needed to recover predictability in the factorization formula. A system of evolution equations for the TMD case was developed by Collins, Soper
and Sterman (CSS) and has been successfully applied to specific processes [240, 241, 273].
A complete treatment of TMD-factorization involves soft gluons, which give rise to an extra "soft factor" $S(\boldsymbol{q})$ in the factorization formula of Eq. (2.45). The TMD-factorization formula then becomes

$$
\begin{equation*}
d \sigma \sim|\mathcal{H}|^{2} \otimes \Phi\left(x, \boldsymbol{k}_{\perp}\right) \otimes D\left(z, \boldsymbol{P}_{\perp}\right) \otimes S\left(\boldsymbol{h}_{T}\right) \delta^{(2)}\left(\boldsymbol{q}_{T}+\boldsymbol{k}_{\perp}-\boldsymbol{P}_{\perp}-\boldsymbol{h}_{T}\right) . \tag{2.49}
\end{equation*}
$$

The soft factor describes the role of gluons with nearly zero center-of-mass rapidity. One difficulty with the usual presentation of the CSS formulation is that the explicit appearance of a soft factor seems somewhat counter to the basic parton model intuition wherein all nonperturbative effects are associated with functions for each external hadron with simple and specific probabilistic interpretations. A natural hope is that, with an appropriate sequence of redefinitions, the role of the soft gluons can be absorbed into the definitions of the PDFs and FFs. The recent work of Collins [384 has shown how this is possible. Indeed, this treatment of the soft factor is necessary for a completely correct factorization derivation with fully consistent definitions for the correlation functions.

While the CSS formalism has been implemented for specific spin independent processes (see, for example, [385]), much work remains to be done in tabulating and classifying the TMDs. This is especially true for cases that involve spin. Work in this direction has been started in [260].

## TMD-factorization breaking

The discussion has focussed on situations where factorization is known to hold. There are also, however, situations where TMD-factorization is now known to break down [265, 267, 268, 270, 271, 272, 381, 382. The key issue is the failure of the usual Ward identity arguments that ordinarily allow eikonalized gluons to be factorized and identified with a particular gauge-link structure in the definitions of the TMDs. A hint of what leads to TMD-factorization breaking is already suggested by the well-known overall relative sign flip in the Sivers function for SIDIS as compared to the Drell-Yan (DY) process [261, 262. The difference comes because in the SIDIS TMD-factorization formula, the gauge link in the Sivers function is future pointing, whereas it is past pointing in the DY case. At the level of Feynman graphs, the difference can be seen in the fact that the "extra" gluons which contribute to the gauge-link attach before the hard scattering in one case, and after the hard scattering in the other. This illustrates that the direction of the flow of color through the eikonal lines is a critical factor in the definition of the correlation functions.

In the more complicated hadro-production processes, $H_{1}+H_{2} \rightarrow H_{3}+H_{4}+X$, where $H_{3}$ and $H_{4}$ may be either jets or hadrons, a reasonable first approach would be to trace the flow of color through the eikonal factors and use analogous arguments to what we used for SIDIS and DY in the previous section. One finds that the resulting structures are not simply the future or past pointing gauge-links familiar from SIDIS or DY, but rather are complicated and highly process dependent objects [265, 267, 381, 382]. That this corresponds (at least) to a breakdown of universality is most directly seen in an explicit spectator model calculation. For example, one may consider an Abelian scalar-quark / Dirac spectator model with multiple flavors as in [270]. Then, in addition to the standard gauge-link attachments, there are extra gluon attachments that do not cancel in a simple Ward identity argument, and which give contributions that are not consistent with having a simple gauge-link like what is found SIDIS or DY (opposite pointing).

Therefore, it is clear that there is at least a violation of universality in the hadroproduction of hadrons. The natural next approach to try is to maintain a basic factorization structure, but to loosen the requirement that the TMDs be universal, resulting in a kind of "generalized" TMD-factorization formalism. That is, the cross section might still be expected to factorize order-by-order into a hard part and well-defined, albeit non-universal, matrix elements for each separate external hadron [268]. However, a careful order-by-order consideration of multiple gluons in the derivation of TMD-factorization shows that even this is not possible [272]. If, for example, one extends the model of [270] to allow the gluons to carry color (while still considering a hard part that involves only the exchange of a colorless boson) then it is straightforward to see that the flow of color spoils the possibility of factorizing the graph into TMD PDFs with separate gauge-links for each TMD, regardless of what kind of gauge-link geometries are allowed. Therefore, the problem with factorization in the hadro-production of hadrons is more than just a problem with universality - separate correlation functions cannot even be defined in a way that is consistent with factorization.

The root of the problem is a failure of Ward identity arguments, which normally allow "extra" gluons to be factorized after a sum over graphs. The Ward identity arguments are only valid after an appropriate sequence of contour deformations on the momentum integrals. In the case of hadro-production of hadrons the necessary deformations are prohibited. In other cases where the direction of color flow may at first appear to pose a problem for factorization (such as in $e+p \rightarrow h_{1}+X$ and $e+p \rightarrow h_{1}+h_{2}+X$ ), the necessary contour deformations are possible and factorization holds. (See the explanation in chapter 12 of 384.)

To summarize, we list the status of TMD-factorization for various well-known processes with a check mark for processes where factorization appears to be valid and !! where it has been shown to fail:
$\checkmark$ Semi-inclusive DIS $\left(e+p \rightarrow e^{\prime}+h_{1}+X\right)$.
$\checkmark$ Drell-Yan (up to overall minus signs for some spin-dependent TMDs).
$\checkmark$ Back-to-Back hadron or jet production in $e^{+} e^{-}$annihilation.
$\checkmark$ Back-to-back hadron or jet production in DIS $\left(e+p \rightarrow e^{\prime}+h_{1}+h_{2}+X\right)$.
!! Hadro-production of back-to-back jets or hadrons $\left(H_{1}+H_{2} \rightarrow H_{3}+H_{4}+X\right)$.
In cases where TMD-factorization is valid, there is still much work left to be done (and much potential insight to be gained) in terms of implementing the evolution of precisely defined TMDs [260]. Much already exists for the case of unpolarized scattering, but even here the most complete and formal identification of evolution effects with separate TMDs has only recently been clarified in [384]. For polarization dependent functions, it is also important to include evolution, but to date there has been very little work that accounts for evolution in actual fits to data.

Finally, the experimental search for TMD-factorization breaking effects opens the possibility of new and exciting insights into the transverse dynamics of hadronic collisions. The breakdown of TMD-factorization in the hadro-production of hadrons implies that unexpected and exotic correlations between partons in different hadrons can exist. Calculations that allow for experiments to distinguish between factorization and factorization-breaking scenarios are therefore very important, and a quantitative understanding of factorization (via the methods of [283], for example) are part of the next step toward understanding hadronic structure in high energy collisions.

### 2.4.2 Evolution of transverse-momentum-dependent densities

Much of the success of QCD collinear factorization relies on our ability to calculate the short-distance partonic dynamics in QCD perturbation theory order-by-order in powers of $\alpha_{s}$ and the universality as well as the scale evolution of the non-perturbative collinear parton distribution and correlation functions. With its dependence on the parton's transverse momentum, TMDs carry much richer information on the partonic structure of a hadron than what collinear PDFs could provide. Like the case of collinear factorization, the predictive power of the TMD factorization formalism also requires our ability to calculate the short-distance dynamics and the evolution of TMDs. However, the theoretical framework for calculating the evolution of TMDs and radiative corrections to short-distance dynamics has not been fully established. All existing parameterizations of TMDs are extracted from SIDIS data at relatively low $Q^{2}$. The available hard scale $Q^{2}$ at a future EIC is expected to be much larger. The TMDs, like PDFs, depend on the momentum scale $Q^{2}$ where they are probed. Understanding the $Q^{2}$ dependence of the TMDs is crucial for testing the TMD factorization formalism and for extracting correct information on the partonic structure of hadrons at the EIC. However, the $Q^{2}$-dependence of TMDs in the existing TMD factorization formalism is very different from the factorization scale $\mu_{F}^{2}$ dependence of the PDFs. The factorization scale is not a physical scale. Any factorized physical cross section should not be sensitive to the choice of the factorization scale. The perturbatively calculated factorization scale dependence of PDFs is necessarily compensated by the same scale dependence in the high order short-distance partonic dynamics. On the other hand, the TMDs in the existing proved TMD factorization formalism are effectively physical quantities. They are connected to a physical observable by a partonic scattering cross section without strong interaction and a soft factor which can be absorbed into the redefinition of TMDs [384. Unlike the DGLAP evolution equation of PDFs, the $Q^{2}$-dependence of TMDs cannot be derived by a simple renormalization group equation. The $Q^{2}$-dependence of TMDs was systematically studied in the context of the transverse momentum $\left(q_{T}\right)$ distribution of the Drell-Yan process and the two-jet momentum imbalance in $e^{+} e^{-}$collisions [273]. The $Q^{2}$-dependence was derived by resumming $\ln ^{2}\left(Q^{2} / q_{T}^{2}\right)$-type large logarithms perturbatively in the impact parameter $b_{T}$-space (a Fourier transform of the parton's transverse momentum space). The CSS formalism was extended to SIDIS [386, 387, as well as spin observables [257, 388]. With the proof that the soft factor of the TMD factorization formalism could be absorbed into the redefinition of TMDs [384, the CSS resummation formalism was recently applied to the TMDs directly [260]. Within the CSS formalism, it is not the $Q^{2}$-dependence of TMDs that is derived but rather the $Q^{2}$-dependence of the Fourier transformed TMDs at small $b_{\perp}$. In order to obtain the $Q^{2}$-dependence of TMDs, one has to perform the Fourier transform from the impact parameter $b_{\perp}$-space to the parton's transverse momentum $k_{T}$-space. The procedure of Fourier transform requires necessarily input from the nonperturbative large $b_{\perp}$ region, which could significantly reduce the predictive power of the TMDs [389]. Various treatments/models for the extrapolation into the large $b_{\perp}$ region have been proposed to fit the existing data [385]. For the precision study of TMDs at the EIC, it is very important to examine the universality of the nonperturbative extrapolation to the large $b_{\perp}$ region and its dependence on the observed kinematic variables; and most important, the predictive power of the formalism [389]. In order to understand the $Q^{2}$-dependence of spin-dependent TMDs, a careful generalization of the CSS resummation formalism to $\boldsymbol{k}_{\perp}$-dependent TMDs is needed [388], which is necessary for the study of asymmetries generated by the TMDs at the EIC.

### 2.4.3 QCD Evolution for the Correlation Functions

As introduced in Sec. [2.2, a collinear factorization formalism at twist-3 is relevant for describing the SSAs of high $P_{h T}$ particle production. Even though the phenomenological applications of this approach have been successful, the theoretical calculations so far have been mainly limited to the "bare" parton model, that is, to the zeroth order of perturbation theory without any QCD corrections. These leading order (LO) calculations have some disadvantages: they strongly depend on the choice of the renormalization as well as the factorization scale, while the physically observed SSAs should not depend on the choice of these scales. The strong dependence on the choice of these scales is an artifact of the LO perturbative calculation, and a significant cancellation of the scale dependence between the leading and the next-to-leading (NLO) contribution is expected from the QCD factorization theorem. As demonstrated by many examples, NLO contributions are typically very important in hadronic processes, and often offer a more comprehensive test of the relevant QCD factorization formalism.

To move forward to the NLO QCD dynamics, it is necessary to study the evolution (or the scale dependence) of the universal long distance distributions and to evaluate the perturbative short-distance contribution beyond the LO. The evolution equation of the twist-3 distribution functions have been derived by different groups [290, 291, 390, 391]. Recently the evolution equations for the twist-3 fragmentation functions have also become available [392]. A first NLO calculation for the short-distance hard part function has been presented in [291].

As emphasized in Sec. 2.3, there are close connections between the twist-3 collinear factorization formalism and the TMD factorization formalism. The twist-3 correlation functions are closely related to the relevant TMD functions. Even though the Collins-Soper evolution equations have been derived for all the leading-twist TMD functions [393, these evolution equations are available in $b$-space ( $b$ is conjugate to the transverse momentum $k_{\perp}$ ). How these evolution equations are transformed into the scale (or energy) dependence of the SSAs (thus leading to a similar Collins-Soper-Sterman transverse momentum resummation) is not yet fully understood.

The evolution equations of twist-3 distribution functions, particularly for the so-called soft-gluonic-pole correlation functions have been derived in [290, 291, 390, 391. Among them, $T_{F}\left(x_{1}, x_{2}\right)$ and $T_{F}^{(\sigma)}\left(x_{1}, x_{2}\right)$ are the most discussed ones and they are related to the Sivers and Boer-Mulders functions [264:

$$
\begin{align*}
T_{F}(x, x) & =-\left.\int d^{2} k_{\perp} \frac{\left|\boldsymbol{k}_{\perp}\right|^{2}}{M_{p}} f_{1 T}^{\perp}\left(x, k_{\perp}^{2}\right)\right|_{\mathrm{DIS}}, \\
T_{F}^{(\sigma)}(x, x) & =-\left.\int d^{2} k_{\perp} \frac{\left|\boldsymbol{k}_{\perp}\right|^{2}}{M_{p}} h_{1}^{\perp}\left(x, k_{\perp}^{2}\right)\right|_{\mathrm{DIS}}, \tag{2.50}
\end{align*}
$$

where $M_{p}$ is the nucleon mass. The evolution equations for both $T_{F}(x, x)$ and $T_{F}^{(\sigma)}(x, x)$ have the following generic form:

$$
\begin{equation*}
\frac{\partial T\left(x, x, \mu^{2}\right)}{\partial \ln \mu^{2}}=\frac{\alpha_{s}}{2 \pi} \int \frac{d x^{\prime}}{x^{\prime}}\left[A(\hat{\xi}) T\left(x^{\prime}, x^{\prime}, \mu^{2}\right)+B\left(x, x^{\prime}\right) T\left(x, x^{\prime}, \mu^{2}\right)\right], \tag{2.51}
\end{equation*}
$$

where $T$ represents either $T_{F}$ or $T_{F}^{(\sigma)}$, and $\hat{\xi}=x / x^{\prime}$. As can be seen in (2.51), the evolution equation for the diagonal correlation function $\left(x_{1}=x_{2}=x\right)$ is not a closed equation since it also depends on the off-diagonal piece (the $B\left(x, x^{\prime}\right)$ term). The diagonal $A(\hat{\xi})$ terms are typically similar to the relevant twist-2 splitting kernel: for $T_{F}$, it is the same as the $q \rightarrow q$
splitting kernel for the unpolarized distribution functions; for $T_{F}^{(\sigma)}$, it is the same as the splitting kernel for the transversity distribution. It might be worth pointing out that there are some discrepancies for the evolution equation of $T_{F}$ in the literature: Ref. 391 contains additional contributions compared to [290, 291, 390]. One additional piece corresponds to a contribution from the mixing between a gluon state and quark-antiquark state, which are missing in [290, 291, 390] and could be easily reproduced. Another term [ $-N_{c} T_{F}(x, x)$ ] seems difficult to reconcile at the moment, and further study is needed to resolve this discrepancy.

Similarly, one could study the evolution of the three-gluon correlation functions. For an initial effort, see [390]. They receive contributions from themselves, as well as from the quark-gluon correlation functions $T_{F}$. Even though our information on three-gluon correlation functions is very scarce, one can not rule out the possibility that they might be large since they could be generated through the QCD radiation from the quark-gluon correlation. It is also worth pointing out that we now have data from PHENIX on the SSA of $J / \Psi$ [313], which turns out to be non-zero and gives some indication that three-gluon correlation functions might be sizable. It has been suggested that open charm production in a future Electron Ion Collider (EIC) with broader kinematics could be used to unravel the three-gluon correlation functions.

Within the same method, one could study the evolution equations for the twist-3 fragmentation functions. The two most important ones are related to the first transverse-momentum-moment of the Collins function $H_{1}^{\perp}\left(z, z^{2} k_{\perp}^{2}\right)$ and the polarizing fragmentation function $D_{1 T}^{\perp}\left(z, z^{2} k_{\perp}^{2}\right)$ [297, 394]:

$$
\begin{equation*}
\hat{H}(z)=-z^{3} \int d^{2} k_{\perp} \frac{\left|\boldsymbol{k}_{\perp}\right|^{2}}{M_{h}} H_{1}^{\perp}\left(z, z^{2} k_{\perp}^{2}\right), \quad \hat{T}(z)=-z^{3} \int d^{2} k_{\perp} \frac{\left|\boldsymbol{k}_{\perp}\right|^{2}}{M_{h}} D_{1 T}^{\perp}\left(z, z^{2} k_{\perp}^{2}\right), \tag{2.52}
\end{equation*}
$$

with both $H_{1}^{\perp}$ and $D_{1 T}^{\perp}$ from the convention in [243]. These twist-3 fragmentation functions belong to the more general two-argument fragmentation functions denoted as $\hat{H}_{F}\left(z, z_{1}\right)$ and $\hat{T}_{F}\left(z, z_{1}\right)$, for details on the operator definitions, see [392]. The evolution equation for $\hat{H}(z)$ takes the following generic form (same form for $\hat{T}(z)$ ):

$$
\begin{equation*}
\frac{\partial \hat{H}\left(z_{h}, \mu^{2}\right)}{\partial \ln \mu^{2}}=\frac{\alpha_{s}}{2 \pi} \int \frac{d z}{z}\left[A(\hat{z}) \hat{H}\left(z, \mu^{2}\right)+\int \frac{d z_{1}}{z_{1}^{2}} \mathrm{PV}\left(\frac{1}{\frac{1}{z}-\frac{1}{z_{1}}}\right) B\left(z_{h}, z, z_{1}\right) \hat{H}_{F}\left(z, z_{1}, \mu^{2}\right)\right] \tag{2.53}
\end{equation*}
$$

where $\hat{z}=z / z_{h}$, and in the case of $\hat{H}\left(z_{h}, \mu^{2}\right), A(\hat{z})$ is the same as the evolution kernel for the transversity distribution; while for $T\left(z_{h}, \mu^{2}\right), A(\hat{z})$ is the same as the $q \rightarrow q$ splitting kernel for the unpolarized fragmentation function.

We have reviewed the evolution equations for the twist-3 distribution and fragmentation functions. Particularly for those related to the first transverse-momentum-moment of the Sivers and Boer-Mulders function, and Collins and polarizing fragmentation function. These evolution equations are generally not a closed set of equations. However, the diagonal pieces are very similar to those appearing in the evolution of leading-twist distribution and fragmentation functions. For the Sivers function and polarizing fragmentation function, this piece is the same as for the unpolarized distribution functions. For the Boer-Mulders function and Collins function, this piece is the same as for transversity. The evolution equations of these functions will transform into the scale dependence of the spin observables, which could be studied at EIC. With a wide coverage in $x$ and $Q^{2}$, EIC offers a great opportunity to study these scale dependences - a direct test of QCD dynamics.

### 2.4.4 Non-perturbative studies of TMDs in effective approaches

TMDs are matrix elements of certain non-local QCD light-front operators in hadron states and can only be calculated using non-perturbative frameworks. Several low-energy QCD-inspired models have been employed. Although they all have in common that they strongly oversimplify the complexity of the QCD dynamics in hadrons, studies in different models based on often complementary assumptions, help to unravel non-perturbative aspects of TMDs. Insights into non-perturbative properties are of particular interest when confirmed in various models. The practical value of model results is that they can be used to predict new observables, or to guide educated Ansätze for fits of TMD parameterizations. Especially in the context of TMDs one should not underestimate the conceptual importance of model calculations. Model calculations demonstrated the existence of effects [261, paved the way towards an understanding of universality in the fragmentation process [395], established new TMDs [396, 397, see [398 for a review. The distinction of T-even and T-odd TMDs is important also from the point of view of modeling. In order to model the former it is sufficient to use a model with explicit quark degrees of freedom. In contrast, the modeling of T-odd TMDs requires the explicit presence of gauge-field degrees of freedom.

In the following we will briefly review TMD models, though a detailed classification of all models in which TMDs have been studied would go far beyond the scope of this section.

## Models of TMDs

An interesting model is QCD in the multicolor limit, i.e. one works with $N_{c} \rightarrow \infty$ instead of $N_{c}=3$ colors. In the large- $N_{c}$ limit the nucleon can be described as a classical soliton of the chiral field [399]. Also for $N_{c} \rightarrow \infty$ QCD cannot be solved (in $3+1$ dimensions). But certain symmetry properties of the soliton field are known [399] and can be used to derive relations which compare the relative magnitudes of different flavor combinations 334,

$$
\begin{align*}
\left(f_{1}^{u}+f_{1}^{d}\right) & \gg\left|f_{1}^{u}-f_{1}^{d}\right|, & & \left|f_{1 T}^{\perp u}-f_{1 T}^{\perp d}\right| \gg\left|f_{1 T}^{\perp u}+f_{1 T}^{\perp d}\right|, \\
\left|g_{1}^{u}-g_{1}^{d}\right| & \gg\left|g_{1}^{u}+g_{1}^{d}\right|, & & \left|g_{1 T}^{\perp u}-g_{1 T}^{\perp d}\right| \gg\left|g_{1 T}^{\perp u}+g_{1 T}^{\perp d}\right|, \\
\left|h_{1}^{u}-h_{1}^{d}\right| & \gg\left|h_{1}^{u}+h_{1}^{d}\right|, & & \left|h_{1 L}^{\perp u}-h_{1 L}^{\perp d}\right| \gg\left|h_{1 L}^{\perp u}+h_{1 L}^{\perp d}\right|, \\
\left|h_{1}^{\perp u}+h_{1}^{\perp d}\right| & \gg\left|h_{1}^{\perp u}-h_{1}^{\perp d}\right|, & & \left|h_{1 T}^{\perp u}-h_{1 T}^{\perp d}\right| \gg\left|h_{1 T}^{\perp u}+h_{1 T}^{\perp d}\right|, \tag{2.54}
\end{align*}
$$

where the not indicated arguments of the TMDs scale with $N_{c}$ as $x \sim 1 / N_{c}$ and $k_{\perp} \sim N_{c}^{0}$. Analogous relations hold for antiquarks (334. In (2.54) the respectively 'large' flavor combinations are one order in $N_{c}$ enhanced compared to the 'small' ones. For known distribution functions the hierarchies in (2.54) are roughly supported in nature 400. The large- $N_{c}$ prediction [334] also proved useful as a guideline for a first extraction of the Sivers function from SIDIS [328]. Conclusions about gluon TMDs can also be drawn. For instance, $f_{1 T}^{\perp g}$ is predicted to be one order in $N_{c}$ suppressed with respect to the quark Sivers distributions [328, which seems supported by phenomenology 401, 402].

The first quark model to give practical results on T-even TMDs was the quark-diquark spectator model 403]. The basic idea of this model is to make a spectral decomposition of the correlation function which defines the TMDs, and to evaluate it in the spectator approximation, i.e. by truncating the sum over intermediate states to a single on-shell spectator with definite mass. The spectator can have the quantum numbers of a scalar (spin 0) isoscalar or axial-vector (spin 1) iso-vector diquark, and it plays the role of an effective particle which effectively takes into account non-perturbative effects related to the
sea and gluon content of the nucleon. The nucleon-quark-diquark coupling is described by an effective vertex which may contain a model-dependent form factor. This class of models with various vertex functions and different choices for the axial-vector diquark polarization states have been used extensively in literature [337, 404, 405, 406]. These results for TMDs can also be interpreted in terms of overlap of light-cone wave functions (LCWFs) for the diquark [407]. The advantage of the spectator model is that the complicated many-particle system can be effectively treated by a simple two-particle technique. However, the price to pay is that basic properties like the momentum and quark-number sum rules cannot be satisfied simultaneously, since the number of quarks "seen" in the spectator model is only one. This fundamental limitation can be resolved only by considering the diquark not as an elementary particle, but as formed by two quarks which play the role of active particles (see, e.g., ref. [408]).

A different approach consists in exploiting LCWFs to model the three-quark structure of the nucleon. The three-quark LCWFs encode the bound state quark properties of hadrons, including their momentum, spin and flavor correlations, in the form of universal processand frame-independent amplitudes. Such amplitudes have also the important property to be eigenstates of the total quark orbital-angular momentum $L_{z}^{q}$ [278, 407] and therefore, allow for mapping in a transparent way the multipole pattern in $\boldsymbol{k}_{\perp}$ associated with each TMD [409, 410. In particular, $f_{1}^{q}, g_{1 L}^{q}$ and $h_{1}^{q}$ describe monopole distributions with $\Delta L_{z}^{q}=0$ between the initial and final nucleon states, with $f_{1}^{q}, g_{1 L}^{q}$ containing $S, P$ and $D$ wave contributions, and $h_{1}^{q}$ only $S$ and $P$ waves. The other twist-2 T-even TMDs are non-diagonal in the orbital angular momentum, with $g_{1 T}^{q}$ and $h_{1 L}^{q}$ describing dipole distributions due to the interference of $S-P$ and $P-D$ waves, and $h_{1 T}^{\perp q}$ being related to a quadrupole shape due to a transfer of two units of orbital angular momentum [411, 301. Two phenomenologically successful models were used to compute the quark LCWFs: the light-cone constituent quark model (LCCQM) 409] and the chiral quark-soliton model ( $\chi$ QSM) 412, 413, 414, 415. In the LCCQM one describes the baryon state in terms of three free on-shell valence quarks. The three-quark state is however not on-shell, i.e. $M \neq \sum_{i} \omega_{i}$, where $\omega_{i}$ is the energy of free quark $i$ and $M$ is the physical mass of the bound state. The motion of the quarks inside the nucleon is described by a momentum-dependent function which is assumed to have a simple analytical expression, with free parameters fitted, e.g., to the anomalous magnetic moments and the axial charge of the nucleon. In the $\chi$ QSM quarks are not free but bound by a relativistic chiral mean field (semi-classical approximation). This field creates a discrete level in the one-quark spectrum and distorts at the same time the Dirac sea. Despite the different model assumptions in LCCQM and $\chi$ QSM, it turns out that the corresponding LCWFs are very similar in structure. It should be noticed that the $\chi \mathrm{QSM}$ naturally incorporates higher Fock states and it has been applied to describe the unpolarized TMD for both quark and antiquarks [416.

A different model used to compute TMDs is the bag model. In its simplest version it describes the nucleon as three non-interacting massless quarks confined inside a sphere. This is therefore the only quark model discussed so far which incorporates confinement, which is modeled by the bag boundary condition, i.e. in some sense the boundary condition mimics gluons [418]. All twist-2 and twist-3 T-even TMDs were studied in this model in 419], and a complete set of linear and non-linear relations among them was derived. Another remarkable insight was that the bag model strongly supports the Gaussian $k_{\perp}$-dependence of TMDs observed in phenomenology [420].

A physical picture nearly "opposite" to the bag model is provided by the covariant


Figure 2.21. Results for $h_{1}^{q}(x)$ (left panels), $h_{1 L}^{\perp(1) q}$ (middle panels) and $h_{1 T}^{\perp(1) q}$ (right panels) as functions of $x$ within different models at low scales for up (upper panels) and down quarks (lower panels). Dashed curves: spectator model of ref. 403. Dotted curves: bag model of ref. 417. Solid curves: light-cone constituent quark model of ref. [298].
parton model 421, 422, 423]. In this approach the partons are free, and assumed to be described in terms of 3D spherically symmetric momentum distributions in the nucleon rest frame. Compliance of the model with relations derived from QCD equations of motion allows the existence of only two such covariant momentum distributions: one describes unpolarized and the other polarized quarks. All twist-2 TMDs are described in terms of these two covariant distributions. This also implies relations among TMDs discussed in [421]. The most interesting aspect of the model is that the symmetry of the covariant momentum distributions tightly connects longitudinal and transverse parton momenta. As a consequence, it is possible to predict the $x$ - and $k_{\perp}$-dependence of TMDs from the $x$ dependence of known PDFs [423]. Interestingly, also this model supports the Gaussian $k_{\perp}$-dependence. An important feature is that the covariant parton model yields results which refer to a large scale. Other parton model approaches in the context of TMDs were discussed in [424, 425, 426].

TMDs in the non-relativistic limit were studied for an arbitrary number of colors $N_{c}$ in [421. In this context we recall the popular non-relativistic model prediction $h_{1}^{q}(x)=g_{1}^{q}(x)$. The non-relativistic model makes similar predictions for other TMDs. In particular, it naturally explains why in many models the integrated pretzelosity function, $h_{1 T}^{\perp q}(x)$, is so large compared to other TMDs.

Results for selected T-even TMDs computed within different models are shown in Fig. 2.21, In order to model T-odd TMDs one needs to invoke also gauge-boson degrees of freedom. We shall devote a separate section to that. But before that we discuss relations among TMDs.

In QCD all TMDs are independent functions. However, in a large class of quark models [409, 403, 405, 413, 414, 415, 419, 421, 422, 423, there appear relations among different TMDs. In fact, certain relations, the so-called 'LIRs' ('Lorentz-invariance relations') must hold in any consistent quark model framework without gauge-field degrees of freedom. The 14 T-even leading- and subleading-twist TMDs can be expressed in terms of 9 independent 'quark-nucleon scattering amplitudes' which implies the relations [243, 427] (see 428] for a review).

## T-odd TMDs

T-odd TMDs emerge from the gauge-link structure of the parton correlation functions which describe initial/final-state interactions (ISI/FSI) via soft-gluon exchanges between the struck parton and the target remnant. Here we will summarize the status of model calculations for the two leading-twist T-odd TMDs, namely the Sivers function $f_{1 T}^{\perp}$ and the Boer-Mulders function $h_{1}^{\perp}$. Both these functions require orbital angular momentum in the nucleon, since they involve a transition between initial and final nucleon states whose orbital angular momentum differ by $\Delta L_{z}^{q}= \pm 1$. Following the first calculation which explicitly predicted a non-zero Sivers function within a scalar-diquark model [261], more refined calculation of the T-odd TMDs were performed in the spectator models with both scalar and axial-vector diquark [337, 404, 429, 430, 431, 432, 433, 434. Other model calculations include the bag model [339, 435, 436], the non-relativistic constituent quark model 437] and a light-cone constituent quark model [298]. Within all these models, the FSI/ISI are approximated by taking into account only the leading contribution due to the one-gluon exchange mechanism. As a result, the final expressions for the T-odd functions are proportional to the strong coupling constant, which plays the role of a global normalization factor with different values depending on the intrinsic hadronic scale of the model. Meanwhile, we also notice that it may be not appropriate to use a perturbative coupling for these non-perturbative calculations. A non-perturbative approach was studied in refs. 438, 439, where T-odd distributions were obtained from the non-perturbative chromomagnetic quarkgluon interaction induced by instantons. A complementary approach is also to take into account the physics of the FSI/ISI by constructing augmented LCWFs which incorporate the rescattering effects by acquiring an imaginary (process-dependent) phase 440. Finally we remark that an interesting way to circumvent the no-go theorem concerning the modeling of T-odd TMDs in chiral quark models [44] was discussed in 333 where the role of gluons is played by a 'hidden vector-meson gauge symmetry'.

Recently, interesting studies were presented, which go beyond the one-gluon exchange approximation by resumming all order contributions [338, 442, 443]. This is achieved using approximate relations between TMDs and GPDs. In particular, the T-odd TMDs are described via factorization of the effects of FSIs, incorporated in a so-called "chromodynamics lensing function", and a spatial distortion of impact parameter space parton distributions [444, 299, 300]. While such relations are fulfilled from lowest order contributions in spectator models [282, 300, they are not expected to hold in general [445, 446]. However, the interesting novelty in the approach of refs. [338, 442, 443] is the calculation of the lensing function using non-perturbative eikonal methods which permit to take into account higher order gluonic contributions from the gauge-link.

A non trivial constraint in modeling or fitting the Sivers function is given by the Burkardt sum rule [447. This sum rule is related to momentum conservation, which requires that the first transverse-momentum moment of the Sivers function, i.e. the net transverse momentum due to final state interactions, should vanish. In the bag model this sum rule is violated by a few percent [339, 435], since the bag states are not good momentum eigenstates. Analogously, the non-relativistic calculation in constituent quark models leads to a small violation of the sum rule. In spectator models, the sum rule is expected to be fulfilled only when taking into account both the quark and the diquark as explicit degrees of freedom 432]. On the other side, it was proven to hold in light-cone constituent quark models [298].

In fig. [2.22 the results from different models for the first transverse-momentum moment of the Sivers and Boer-Mulders functions are compared with phenomenological parametriza-


Figure 2.22. Results for the (1)-moments of the quark Sivers (upper panels) and Boer-Mulders (lower panels) functions as function of $x$. The different curves correspond to the results after (approximate) evolution from the model scale to $Q^{2}=2.5 \mathrm{GeV}^{2}$. Solid curves: light-cone constituent quark model of ref. [298]. Dashed curves: spectator model of ref. [337. Dotted curves: bag model of ref. [339, 436]. In the case of the Sivers function, the lighter and darker shaded areas indicate statistical uncertainties of the parameterizations of ref. [332 and 328, 331. For the Boer-Mulders function the dashed-dotted curves are the results of the phenomenological parametrization of refs. 366, 367.
tions [328, 332, 331, valid at an average scale of $Q^{2}=2.5 \mathrm{GeV}^{2}$, extracted by a fit to available experimental data for pion and kaon production in semi-inclusive deep inelastic scattering. The model results are evolved from the corresponding hadronic scale to $Q^{2}=2.5$ $\mathrm{GeV}^{2}$, by employing those evolution equations which seem most promising to be able to simulate the correct evolution, which is presently not available. In particular, we evolved the (1)-moment of the Sivers function by means of the evolution pattern of the unpolarized parton distribution, while for the (1)-moment Boer-Mulders function we used the evolution pattern of the chiral-odd transversity. Within the large error bar, the results of both the LCCQM and spectator model for the Sivers function are compatible with the parameterizations for both up and down quark, although the shapes of the distributions and the magnitude of the up- and down-quark contributions are quite different. On the other hand, the bag model predicts much smaller results, for both the Sivers and Boer-Mulders functions. In all the models the Boer-Mulders function has the same sign for both the up and down contributions, confirming theoretical expectations [334, 448]. Furthermore, the up and down contributions to the Boer-Mulders function are expected to have the same order of magnitude within the available parametrizations [366, 367, 370, 449. This is confirmed from the predictions of the LCCQM and bag model, while it is at variance with the spectator model where the up distribution is more than twice bigger than the down distribution. However, we note that the available data do not allow yet a full fit of $h_{1}^{\perp}$ with its $x$ and $k_{\perp}^{2}$ dependence and the available phenomenological parameterizations are only first attempts to extract information on this distribution. New experimental data will play a crucial role to better constrain these analyses.

### 2.5 Chiral-odd partonic densities

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Half of the leading-twist TMDs are denoted by the letter $h$, which means that they describe the distribution of transversely polarized partons. In the helicity basis for a spin $\frac{1}{2}$ nucleon, where the unpolarized distribution $f_{1}$ and the helicity distribution $g_{1}$ have their well known probabilistic interpretation, transverse polarization states are given by linear combinations of positive and negative helicity states. Since helicity and chirality are the same at leading twist [245], they are called chiral-odd distributions.

One of the four leading-twist chiral-odd TMDs, the transversity distribution $h_{1}$, survives the integration upon transverse momentum. From the experimental point of view, transversity is quite an elusive object. In any observable the chiral-odd transversity needs to be coupled to a chiral-odd nonperturbative partner. In SIDIS, as discussed in Sec. 2.1, $h_{1}$ can appear in the leading-twist part of the cross section together with the chiral-odd Collins fragmentation function $H_{1}^{\perp}$, which can be determined separately, e.g., by measuring azimuthal asymmetries of the distribution of back-to-back pions in two-jet events in electronpositron annihilations, i.e. $e^{+} e^{-} \rightarrow \pi^{+} \pi^{-} X$ [250, 369]. Another promising approach to access transversity is semi-inclusive production of pion pairs, $e p^{\uparrow} \rightarrow e^{\prime}\left(\pi^{+} \pi^{-}\right) X$ [450, where the chiral-odd partner of $h_{1}$ is represented by the chiral-odd Dihadron Fragmentation Function (DiFF) $H_{1}^{\varangle}$ 451].

Among the remaining chiral-odd quark distributions, the so-called Boer-Mulders function attracted great interest from both experiment and theory. It shares some common features as the quark Sivers function discussed in Sec. 2.2. In this section, we will dedicate one subsection to briefly describe this function, including the unique opportunity of exploring it using unpolarized hadrons.

### 2.5.1 The quark transversity distribution

At leading twist, three collinear distribution functions are needed to describe the quark distribution in the nucleon. Transversity is a leading-twist collinear PDF and enjoys the same status as $f_{1}$ and $g_{1}$ [452, 418. An important difference between $h_{1}$ and $g_{1}$ is that in spin- $\frac{1}{2}$ hadrons there is no gluonic function analogous to transversity. The most important consequence is that $h_{1}^{q}$ for a quark with flavor $q$ does not mix with gluons in its evolution and it behaves as a non-singlet quantity; this has been verified up to NLO, where chiral-odd evolution kernels have been studied so far [453, 454, 455].

The tensor charge of the nucleon is defined as the sum of the Mellin moments $\delta q\left(Q^{2}\right)=$ $\int d x\left[h_{1}^{q}\left(x, Q^{2}\right)-h_{1}^{\bar{q}}\left(x, Q^{2}\right)\right]$. Contrary to the axial charge - which is related to $g_{1}^{q}\left(x, Q^{2}\right)$ - it has a nonvanishing anomalous dimension: it evolves with the hard scale $Q^{2}$ [418]. It has been calculated on the lattice [456] and in various models [408, 457, 458, 459, 460], and was found to be sizable. For a more comprehensive review, we refer to Ref. 461.

The extraction of transversity is of fundamental interest for obtaining a complete description of the nucleon structure even for the case when internal transverse momenta are integrated over. To achieve this goal, it is crucial to cover the widest possible range in $\left(x, Q^{2}\right)$, to measure the related asymmetries differential in the relevant kinematic variables and to be able to perform a flavor separation.

| experiment (laboratory) | $\sqrt{s}$ in GeV | target type | hadron types | references |
| :--- | :---: | :---: | :---: | :---: |
| COMPASS (CERN) | 18 | deuteron | $h^{ \pm}, \pi^{ \pm}, K^{ \pm}, K^{0}$ | [320, [321] |
|  |  | proton | $h^{ \pm}$ | [322] |
|  |  | proton | $\pi^{ \pm}, K^{ \pm}$ | prelim. [323] |
| HERMES (DESY) | 7.4 | proton | $\pi^{ \pm}$ | $[324]$ |
|  |  | proton | $\pi^{ \pm}, \pi^{0}, K^{ \pm}$ | $462]$ |
| HallA (JLab) | 3.5 | neutron | $\pi^{ \pm}$ | prelim. [326] |

Table 2.4. Summary of currently available measurements of Collins asymmetry amplitudes from lepton-nucleon DIS experiments, their center-of-mass energy, transversely polarized target type, and analyzed hadron types.

## The Collins effect

As discussed in Sec. 1, at tree-level and leading-twist, the SIDIS $F_{U T}^{\sin \left(\phi_{h}+\phi_{S}\right)}$ structure function of Eq. (2.8) can be described as a convolution between the transversity $h_{1 T}^{q}$ and the Collins fragmentation function $H_{1}^{\perp q}$, i.e.,

$$
\begin{equation*}
F_{U T}^{\sin \left(\phi_{h}+\phi_{S}\right)} \sim \sum_{q} e_{q}^{2} h_{1 T}^{q} \otimes H_{1}^{\perp q} \tag{2.55}
\end{equation*}
$$

In order to project out the structure function $F_{U T, T}^{\sin \left(\phi_{h}+\phi_{S}\right)}$ in Eq. (2.8), the so-called Collins amplitude $2\left\langle\sin \left(\phi_{h}+\phi_{S}\right)\right\rangle_{U T}^{h}$ for a specific hadron $h$ is extracted from the asymmetry

$$
\begin{equation*}
A_{U T}^{h}\left(\phi_{h}, \phi_{S}\right) \equiv \frac{1}{\left|\mathbf{S}_{T}\right|} \frac{d \sigma^{h}\left(\phi_{h}, \phi_{S}\right)+d \sigma^{h}\left(\phi_{h}, \phi_{S}+\pi\right)}{d \sigma^{h}\left(\phi_{h}, \phi_{S}\right)+d \sigma^{h}\left(\phi_{h}, \phi_{S}+\pi\right)}, \tag{2.56}
\end{equation*}
$$

where the subscript $U$ indicates an unpolarized lepton beam and $T$ a transversely polarized target nucleon. The azimuthal angles are illustrated in Fig. 2.1. This amplitude has so far been extracted by three polarized fixed-target experiments as summarized in Table 2.4 . From these measurements, Fig. 2.23 shows a selection of results that are significantly nonzero and help in determining both the shape of transversity and the relative size and sign of the Collins fragmentation function. All other asymmetry amplitudes listed in Table 2.4 are small or consistent with zero.

For the second unknown in Eq. (2.55), the Collins fragmentation function, model calculations are available [382, 463, 464, 465, 466, 467, 468, 469]. However, for a modelindependent extraction of transversity from the SIDIS asymmetry amplitudes we need to determine the Collins function from an independent source. This is represented by the measurement of azimuthal asymmetries in the distribution of back-to-back pions in two-jet events in electron-positron annihilations, i.e. $e^{+} e^{-} \rightarrow \pi^{+} \pi^{-} X 470$.

The relevant vectors and angles involved in $e^{+} e^{-}$annihilations leading to back-to-back jets are depicted in Fig. 2.24 (left panel). The following asymmetry can be measured [250, 369

$$
\begin{equation*}
A_{12}\left(z_{1}, z_{2}, \theta_{2}, \phi_{1}+\phi_{2}\right)=1+\frac{\sin ^{2} \theta}{1+\cos ^{2} \theta} \cos \left(\phi_{1}+\phi_{2}\right) \frac{\sum_{q} e_{q}^{2} H_{1}^{\perp(1) q}\left(z_{1}\right) H_{1}^{\perp(1) \bar{q}}\left(z_{2}\right)}{\sum_{q} e_{q}^{2} D_{1}^{q}\left(z_{1}\right) D_{1}^{\bar{q}}\left(z_{2}\right)} . \tag{2.57}
\end{equation*}
$$



Figure 2.23. Collins amplitudes for $\pi^{+}, \pi^{-}$and $K^{+}$(as denoted in the panels) from HERMES 462 and COMPASS 323 measured with a proton target. Inner error bars present statistical uncertainties and full error bars the quadratic sum of statistical and systematic uncertainties. Note that the average kinematics in each bin differs for HERMES and COMPASS and the sign of the COMPASS asymmetries have been reversed.

Pioneering measurements of this spin-dependent fragmentation function have been performed by the BELLE Collaboration (KEK) 472, 471. Experimentally, double ratios of asymmetries for like-sign (L), unlike-sign (U) and any charged (C) pion pairs are built in order to cancel (to a large extent) contributions from the experimental acceptance and radiative effects. The resulting asymmetries, $A^{U L}$ and $A^{U C}$, are then sensitive to different combinations of the favored and unfavored Colllins fragmentation functions as given in [471]. These asymmetries are presented in Fig. [2.24 as function of $z_{2}$ for four bins of $z_{1}$ for the light quarks $(u, d, s)$, where $z_{1}$ and $z_{2}$ are for a hadron in each of the back-to-back jets.

The experimental results shown in Figs. 2.23 and 2.24 are striking. First, they clearly demonstrate that the Collins effect as a manifestation of chiral-odd and naïve T-odd mechanisms is different from zero and not suppressed, both in SIDIS and in $e^{+} e^{-}$annihilations. Second, the results for oppositely charged pions (hadrons) in Fig. 2.23 suggest a very peculiar feature for the Collins fragmentation function. As scattering off $u$ quarks dominates these data due to the charge factor, the large magnitude of $\pi^{-}$amplitudes being of similar size than the $\pi^{+}$ones but having opposite sign, can only be understood if the disfavored Collins function $H_{1}^{\perp}$ unfav is large and of opposite sign to the favored one. Opposite signs for the favored and unfavored Collins functions are also supported by the different size of $A^{U L}$ and $A^{U C}$ asymmetries from BELLE in Fig. 2.24. They can be understood in light of the string model of fragmentation [463] (and also of the Schäfer-Teryaev sum rule [473). If a favored pion is created at the string end by the first break, an unfavored pion from the


Figure 2.24. Left: the kinematics of $e^{+} e^{-}$annihilation leading to back-to-back jets along the $\hat{\boldsymbol{z}}$ axis (jet frame), $P_{1}$ is the momentum of a hadron in one jet, $P_{2}$ is the momentum of a hadron in the other jet. Right: Collins asymmetry $A_{12}$ for the double ratios for like-sign (L), unlike-sign (U) and any charged (C) pion pairs as function of $z_{2}$ in bins of $z_{1}$ from BELLE 471. $A^{U L}$ and $A^{U C}$ are sensitive to different combinations of the favored and unfavored Collins fragmentation functions.
next break is likely to inherit transverse momentum in the opposite direction.
The extraction of transversity and Collins functions from available data faces the same issues as discussed for the Sivers function in Sec. 2.2 .1 for resolving the convolution in Eq. (2.55) and the same strategies are applied here. Employing the Gaussian Ansatz in Eq. (2.22) both transversity and Collins function have been extracted [250, 474] from (part of) the experimental data discussed before. The new COMPASS proton or Hall-A neutron data are not yet included in this fit. The results of this global analysis are presented in Fig. 2.25 for $u$ and $d$ transversity distributions (left panel) and favored and unfavored Collins fragmenation functions (right panel). The decrease in the presented uncertainties for the specifically chosen parametrization, which is the same as in [250, 474], is due to the new BELLE and HERMES data. The extracted favored and unfavored Collins functions confirm the features discussed before.

## Dihadron Fragmentation Functions

A complementary approach to transversity is provided by semi-inclusive two-hadron production, $e p^{\uparrow} \rightarrow e^{\prime}\left(h_{1} h_{2}\right) X$, where the two unpolarized hadrons with momenta $P_{1}$ and $P_{2}$ emerge from the fragmentation of the struck quark. The underlying mechanism differs from the Collins mechanism in that the transverse spin of the fragmenting quark is transferred to the relative orbital angular momentum of the hadron pair. Consequently, this mechanism does not require transverse momentum of the hadron pair and collinear factorization applies.

Dihadron fragmentation functions were introduced in Ref. [475] and studied for the polarized case in Refs. [450, 476, 477]. The decomposition of the SIDIS cross section in terms of quark distributions and dihadron fragmentation functions was carried out to leading twist in Ref. 451 and to sub-leading twist in Ref. [478].

The kinematics is similar to the one in single-hadron SIDIS except for the final hadronic


Figure 2.25. Left: transversity $x h_{1}^{q}(x)$ for $u$ (upper panel) and $d$ (lower panel) quarks. Right: the normalized Collins functions $\sqrt{2} H_{1}^{\perp(1 / 2)}(z) / D_{1}(z)$ for favored (upper panel) and unfavored (lower panel) fragmentation. The light grey band represents the uncertainty for the extraction in Ref. 250 and the dark grey band from the updated analysis 474. Blue lines indicate the Soffer and positivity bound for transversity and Collins function, respectively.
state, where now $z=z_{1}+z_{2}$ is the fractional energy carried by the hadron pair and we introduce the vectors $P_{h}=P_{1}+P_{2}$ and $R=\left(P_{1}-P_{2}\right) / 2$ (see Fig. 2.26), together with the pair invariant mass $M_{h}$, which must be considered much smaller than the hard scale (e.g., $P_{h}^{2}=M_{h}^{2} \ll Q^{2}$ ). We shall often use the quantity [479],

$$
\begin{equation*}
|\boldsymbol{R}|=\frac{1}{2} \sqrt{M_{h}^{2}-2\left(M_{1}^{2}+M_{2}^{2}\right)+\left(M_{1}^{2}-M_{2}^{2}\right)^{2}} \tag{2.58}
\end{equation*}
$$

where $P_{1}^{2}=M_{1}^{2}, P_{2}^{2}=M_{2}^{2}$ and $R_{T}^{2}$ is related to $M_{h}^{2}$ [479].
In analogy with the Collins function, the expression for unpolarized hadrons ( $h_{1}, h_{2}$ ) produced by a transversely polarized quark reads

$$
\begin{equation*}
D_{h_{1} h_{2} / q^{\uparrow}}\left(z, M_{h}^{2}, \boldsymbol{R}_{T}\right)=D_{1}^{q}\left(z, M_{h}^{2}\right)-H_{1 s p}^{\Varangle q}\left(z, M_{h}^{2}\right) \frac{\boldsymbol{S}_{\perp q} \cdot\left(\hat{\boldsymbol{p}} \times \boldsymbol{R}_{T}\right)}{M_{h}} \tag{2.59}
\end{equation*}
$$

Choosing $\hat{\boldsymbol{p}} \| \hat{z}$ and $\boldsymbol{S}_{\perp q} \| \hat{y}$, a positive $H_{1 s p}^{\Varangle q}$ means that hadron $h_{1}$ is preferentially emitted along $-\hat{x}$ and hadron $h_{2}$ along $\hat{x}$.

Since $\boldsymbol{R}_{T}=\boldsymbol{R} \sin \theta$, where in the c.m. frame of the hadron pair $\theta$ is the angle between $P_{1}$ and the direction of $P_{h}$ in the laboratory frame (for more details, see refs. 479, 480, 481, [482]), the relevant asymmetry that should be measured in SIDIS is

$$
\begin{align*}
A_{U T}^{\sin \left(\phi_{R}+\phi_{S}\right) \sin \theta} & \equiv 2 \frac{\int d \cos \theta d \phi_{R} d \phi_{S} \sin \left(\phi_{R}+\phi_{S}\right)\left[d \sigma\left(\phi_{R}, \phi_{S}\right)-d \sigma\left(\phi_{R}, \phi_{S}+\pi\right)\right] / \sin \theta}{\int d \cos \theta d \phi_{R} d \phi_{S}\left[d \sigma\left(\phi_{R}, \phi_{S}\right)+d \sigma\left(\phi_{R}, \phi_{S}+\pi\right)\right]} \\
& \sim \frac{|\boldsymbol{R}|}{M_{h}} \frac{\sum_{q} e_{q}^{2} h_{1}^{q}(x) H_{1 s p}^{\Varangle q}\left(z, M_{h}^{2}\right)}{\sum_{q} e_{q}^{2} f_{1}^{q}(x) D_{1}^{q}\left(z, M_{h}^{2}\right)} . \tag{2.60}
\end{align*}
$$

As in the single-hadron production case, transversity can be extracted from the asymmetry (2.60) only if the unknown $H_{1 s p}^{\Varangle}$ is independently determined from the $e^{+} e^{-}$annihilation producing, in this case, two hadron pairs: $e^{+} e^{-} \rightarrow\left(\pi^{+} \pi^{-}\right)_{\text {jet } 1}\left(\pi^{+} \pi^{-}\right)_{\text {jet2 }} X$ with kinematics


Figure 2.26. Kinematics for the production of two hadrons (left) and for the $e^{+} e^{-} \rightarrow$ $\left(\pi^{+} \pi^{-}\right)_{\text {jet1 }}\left(\pi^{+} \pi^{-}\right)_{\text {jet2 }} X$ process (right).
depicted in Fig. 2.26 (right). The relevant signal is similar to that of the Collins function, except that each transverse polarization of the quark-antiquark pair is now correlated to the azimuthal orientation of the plane formed by the momenta of the corresponding hadron pairs, suggesting that $H_{1}^{\varangle}$ is related to the concept of handedness of the jet containing a specific pair 483, 484, 485.

The leading-twist cross section of this process contains many terms [485], among which there is one involving the product of $H_{1 s p}^{\Varangle q}$ for the quark $q$ and of $\bar{H}_{1 s p}^{\Varangle q}$ for the $\bar{q}$ partner, weighted by $\cos \left(\phi_{R}+\bar{\phi}_{R}\right)$. Thus, we can properly weight the cross section and extract this contribution by defining the so-called Artru-Collins azimuthal asymmetry [485, 482
$A^{\cos \left(\phi_{R}+\bar{\phi}_{R}\right)}\left(\cos \theta_{2}, z, M_{h}^{2}, \bar{z}, \bar{M}_{h}^{2}\right)=\frac{\sin ^{2} \theta_{2}}{1+\cos ^{2} \theta_{2}} \frac{\pi^{2}}{32} \frac{|\boldsymbol{R}||\overline{\boldsymbol{R}}|}{M_{h} \bar{M}_{h}} \frac{\sum_{q} e_{q}^{2} H_{1 s p}^{\Varangle q}\left(z, M_{h}^{2}\right) \bar{H}_{1 s p}^{\Varangle q}\left(\bar{z}, \bar{M}_{h}^{2}\right)}{\sum_{q} e_{q}^{2} D_{1}^{q}\left(z, M_{h}^{2}\right) \bar{D}_{1}^{q}\left(\bar{z}, \bar{M}_{h}^{2}\right)}$,
where the dihadron fragmentation functions $D_{1}^{q}$ and $H_{1 s p}^{\Varangle q}$ are the same universal functions appearing in the SIDIS asymmetry of equation (2.60).

Pioneering measurements of $A_{U T}^{\sin \left(\phi_{R}+\phi_{S}\right) \sin \theta}$ from HERMES 481] gave evidence for a non-zero dihadron fragmentation function $H_{1 s p}^{\Varangle q}$ as shown in Fig. 2.27. The $M_{h}$ dependence does not exhibit any sign change and rules out the model of Ref. [476]: interference patterns in semi-inclusive $\pi^{+} \pi^{-}$production are different from those in $\pi^{+} \pi^{-}$elastic scattering. Calculations based on the spectator model [480, 486] are compatible with data. They, however, overestimate the asymmetries if $h_{1}^{q}$ is taken from the parametrization 474] discussed in Fig. 2.25. This estimate is presented in Fig. 2.27 by the grey band where the model $H_{1 s p}^{\Varangle q}$ is reduced by a factor $\alpha=0.32 \pm 0.06$ in order to reproduce the magnitude of the asymmetry.

Preliminary SIDIS data are also available from the COMPASS Collaboration using transversely polarized deuteron and hydrogen [487] targets. While $A_{U T}^{\sin \left(\phi_{R}+\phi_{S}\right) \sin \theta}$ is basically vanishing on the deuteron, the proton data show a signal larger than the HERMES results in Fig. 2.27, which might be due to different kinematics.

Last but not least, results from pioneering measurements of the $A^{\cos \left(\phi_{R}+\bar{\phi}_{R}\right)}$ asymmetry related to the dihadron fragmentation function became recently available from the BELLE


Figure 2.27. The spin asymmetry for the semi-inclusive production of a pion pair in deep-inelastic scattering on a transversely polarized proton 481. The grey band presents a fit to the data involving the dihadron FF calculated in the spectator model of Ref. [480] and on the parametrization for $h_{1}$ from Ref. 474.

Collaboration in Ref. 488.
For a real breakthrough of this promising approach to transversity, much more data over wide kinematic range are needed. We only mention that the SIDIS cross section does now depend on nine kinematic variables compared to six for the single-hadron case, which calls even more for a multi-dimensional analysis for a bias-free extraction of the asymmetries.

## Collins effect at EIC

The exploration of chiral-odd structures using the Collins effect is far from being complete. Several aspects need to be significantly improved. The $x$ dependence is largely unconstrained due to the lack of SIDIS asymmetries outside the range $0.005 \lesssim x \lesssim 0.3$. The antiquark and sea-quark content of transversity in the proton is completely unknown. Together with the loose constraints on the $x$ dependence, this missing piece of information makes the calculation of the tensor charge still unsatisfactory. Also the transverse momentum dependence of both the transversity and the Collins function has a significant degree of arbitrariness. Lastly, the $Q^{2}$ range of HERMES and COMPASS measurements is approximately the same: it would be desirable to study the $A_{U T}^{\sin \left(\phi_{h}+\phi_{S}\right)}\left(Q^{2}\right)$ dependence in a wide range of $Q^{2}$.

All these remarks call for more data in order to enlarge the phase space and perform a multi-dimensional analysis in all relevant kinematic variables simultaneously. An ambitious program is planned at JLab12, that would aim for exploring $A_{U T}^{\sin \left(\phi_{h}+\phi_{S}\right)}$ in the valence region with high luminosity [340, 341]. The EIC would be the ideal facility to carry out this program over a uniquely wide range in $x$ and $Q^{2}$. This potential for a mapping of the multi-dimensional phase-space in an unprecedented kinematic range is illustrated by the studies presented in Sec. 2.2 .2 and are equally valid for transversity.

The promising and complementary approach of extracting transversity with help of the dihadron fragmentation function will even more profit from the high energy option of an EIC. Fig. 2.28 shows the projected accuracy for semi-inclusive kaon pair production at an energy $\sqrt{s}=140 \mathrm{GeV}$ and for an integrated luminosity of $30 \mathrm{fb}^{-1}$. The PYTHIA event generator has been used to obtain the SIDIS event rate, and an overall detection efficiency of $50 \%$ and beam polarization of $70 \%$ were assumed. Data are shown as function of $x$ for the various different $z$ and $M_{K K}$ bins indicated in the panels. The invariant mass range of the kaon pair, $M_{K K}$, is chosen for the vicinity of the $\phi$ meson, which provides unique access


Figure 2.28. Projected accuracy, represented by the error bars, for semi-inclusive kaon pair production obtained with an energy of $\sqrt{s}=140 \mathrm{GeV}$ for an integrated luminosity of $30 \mathrm{fb}^{-1}$, as a function of $x$ in bins in $z, M_{K K}$ and for a single bin in $Q^{2}$ as indicated in the panels.
to strange quark distributions.
Furthermore, the general picture obtained so far would significantly profit from data available over a wide $Q^{2}$ range which can only be provided by the EIC. This picture obtained so far, is based on a tree-level analysis of transverse-momentum dependent azimuthal (spin) asymmetries occurring at very different energies: while the average scale of SIDIS experiments is approximately $2.5 \mathrm{GeV}^{2}$, the BELLE measurement was performed at the typical bottonium mass, i.e. $Q^{2} \sim 100 \mathrm{GeV}^{2}$. Beyond tree level, the evolution effects with running scale were included (at LO) only in the modification of the $x$ and $z$ dependence of the various functions. At low $\boldsymbol{P}_{h T}^{2} / Q^{2}\left(Q_{T}^{2} / Q^{2}\right.$ for $e^{+} e^{-}$annihilation, where $Q_{T}=\left|\boldsymbol{q}_{T}\right|$ is the transverse momentum of the virtual photon), the correct $Q^{2}$ dependence beyond tree level of transverse-momentum dependent structure functions should be studied extending the Collins-Soper-Sterman formalism mentioned in Sec. 2.2.6 [273]. A quantitative attempt to go in this direction was presented in Ref. 369, where it was estimated that transversemomentum resummation produces a suppression of the tree level result by almost a factor 5 at BELLE energies. Therefore, the extraction of the Collins function using the tree level formula could significantly underestimate its actual magnitude. In order to fit the available SIDIS asymmetries, a larger $H_{1}^{\perp}$ would automatically imply a transversity smaller than that one illustrated in Fig. 2.25.

### 2.5.2 Boer-Mulders function

The Boer-Mulders function $h_{1}^{\perp}$ [244] can be considered as the counterpart of the Sivers function $f_{1 T}^{\perp}$ : while $f_{1 T}^{\perp}$ describes the distribution of unpolarized quarks in a transversely polarized target, $h_{1}^{\perp}$ describes the distribution of transversely polarized quarks in an unpolarized target. Both functions are T-odd, and therefore vanish if the gauge-link is not taken into account in their operator definition, which makes them somewhat unique among the TMDs. Put it differently, their existence depends on the presence of initial and/or final state interactions between the active partons of a process and the target remnants (see the corresponding discussion in Sec. [2.4.1]. It is expected that both TMDs change their sign when going from SIDIS to the Drell-Yan process [262]. There is, however, one important difference between them. The Sivers function is chiral-even, whereas the Boer-Mulders function is chiral-odd. Since the elementary interactions of the Standard Model do not change the chirality (helicity) of fermions, one has to couple the Boer-Mulders function - like any other chiral-odd object too - to another nonperturbative chiral-odd correlator in order to generate a non-zero observable. This implies that $h_{1}^{\perp}$, in general, is harder to measure than $f_{1 T}^{\perp}$.

On the other hand, in the case of the Boer-Mulders function no polarized target is required, which makes this distribution rather attractive. In fact, it is believed that the Boer-Mulders effect is essential for understanding data on the angular distribution of the unpolarized Drell-Yan process [489]. To be more specific, the general structure of the DrellYan cross section reads (see [490] and references therein)

$$
\begin{equation*}
\frac{1}{\sigma_{D Y}} \frac{d \sigma_{D Y}}{d \Omega}=\frac{3}{4 \pi} \frac{1}{\lambda+3}\left(1+\lambda \cos ^{2} \theta+\mu \sin 2 \theta \cos \phi+\frac{\nu}{2} \sin ^{2} \theta \cos 2 \phi\right), \tag{2.62}
\end{equation*}
$$

where the angles $\theta$ and $\phi$ characterize the orientation of the lepton pair in a dilepton rest frame like the Collins-Soper frame 491. What attracted particular attention is the so-called Lam-Tung relation between the coefficients $\lambda$ and $\nu$ [350, 492],

$$
\begin{equation*}
\lambda+2 \nu=1 \tag{2.63}
\end{equation*}
$$

This relation is exact if one computes the Drell-Yan process to $\mathcal{O}\left(\alpha_{s}\right)$ in the standard collinear perturbative QCD framework. Even at $\mathcal{O}\left(\alpha_{s}^{2}\right)$ the numerical violation of (2.63) is small [493]. However, data for $\pi^{-} N \rightarrow \mu^{-} \mu^{+} X$ taken at CERN [345, 346] and at Fermilab [494] were found to clearly violate the Lam-Tung relation. In particular, an unexpectedly large $\cos 2 \phi$ modulation of the cross section was observed. Various explanations of this experimental result have been put forward, with the most favorable one being based on intrinsic transverse motion of partons leading to the Boer-Mulders effect [489]. The product of two Boer-Mulders functions - one for each initial state hadron - contributes to the $\cos 2 \phi$ term in the cross section in (2.62) (489). An ultimate understanding of the angular distribution in (2.62), and thus also of the role played by the Boer-Mulders function, is of crucial importance if one keeps in mind that, from a theoretical point of view, the Drell-Yan process is the cleanest hard hadron-hadron reaction.

Several model calculations have been carried out for the Boer-Mulders function of both the nucleon [282, 298, 337, 338, 404, 429, 435, 436 and the pion 443, 446, 495], where the treatments for the nucleon comprise spectator models, the MIT bag model, and constituent quark models. In the case of the nucleon two general features emerge: first, the BoerMulders function comes out to be as large as the Sivers function or even larger. Second, it has the same sign for up-quarks and down-quarks. This finding nicely agrees with a
model-independent analysis according to which $h_{1}^{\perp u}=h_{1}^{\perp d}$ to leading order of an expansion in powers of $1 / N_{c}$, with $N_{c}$ being the number of colors [334].

A lot of attention has been paid to an intuitive relation between the Boer-Mulders function and (a specific linear combination of) chiral-odd Generalized Parton Distributions in impact parameter space [496, 497]. (This connection between two types of parton distributions is the analogue of a corresponding relation involving the Sivers function which was proposed earlier [444, 299].) The intuitive picture is compatible with the two general results from model calculations discussed above. In particular, it also suggests a significant size for the Boer-Mulders function in the valence region. In Quantum Field Theory one can make such a relation quantitative in the framework of simple spectator models [282, 433, 300]. However, according to current knowledge, a general model-independent relation cannot exist 445, 446].

The Boer-Mulders function describes the strength of a correlation between the transverse momentum and the transverse spin of the active quark. This correlation generates a dipole pattern in the transverse $k_{\perp}$-plane - like the correlations associated with $f_{1 T}, g_{1 T}$, and $h_{1 L}^{\perp}$ do. One way of visualizing the Boer-Mulders effect is by looking at the density

$$
\begin{equation*}
\rho_{h_{1}^{\perp}}^{q}\left(\boldsymbol{k}_{\perp}, \boldsymbol{s}_{\perp}\right)=\int d x \frac{1}{2}\left[f_{1}^{q}\left(x, \boldsymbol{k}_{\perp}^{2}\right)+\frac{\epsilon_{\perp}^{i j} s_{\perp}^{i} k_{\perp}^{j}}{M} h_{1}^{\perp q}\left(x, \boldsymbol{k}_{\perp}^{2}\right)\right] \tag{2.64}
\end{equation*}
$$

describing the distribution of transversely polarized quarks in an unpolarized nucleon [298]. The quark polarization is specified by the spin vector $s_{\perp}$. Note that the longitudinal momentum fraction has been integrated over. In Eq. (2.64), the $f_{1}$ term provides an axially symmetric contribution, while the second term containing $h_{1}^{\perp}$ gives rise to the mentioned dipole pattern. If both effects are superimposed, the resulting distribution is shifted away from the center (distorted) in the $k_{\perp}$-plane.

The Boer-Mulders function can also be studied in SIDIS and therefore at the EIC. In this process it couples to the chiral-odd Collins fragmentation function $H_{1}^{\perp}$ [249] and gives rise to a $\cos 2 \phi_{h}$-modulation of the cross section. The pertinent structure function takes the generic form

$$
\begin{equation*}
F_{U U}^{\cos 2 \phi_{h}} \sim \sum_{q} e_{q}^{2}\left(h_{1}^{\perp q} \otimes H_{1}^{\perp q}+\frac{C}{Q^{2}} f_{1}^{q} \otimes D_{1}^{q}+\ldots\right) \tag{2.65}
\end{equation*}
$$

where $C$ is a kinematic factor. The second term on the right hand side of (2.65) is the so-called Cahn effect 498, 499, which is also caused by intrinsic transverse parton motion. It is a kinematic twist-4 contribution, i.e., it is suppressed by a factor $1 / Q^{2}$ relative to the first term. Theoretical estimates of this effect are still plagued by large uncertainties, mainly related to the insufficient knowledge of the transverse momentum dependence of $f_{1}^{q}$ and $D_{1}^{q}$. The explicit form of all potential additional (dynamical) twist-4 effects in this structure function is presently not known. These considerations show that a reliable extraction of the Boer-Mulders function from SIDIS requires data in a kinematic region for which the (largely unknown) higher-twist contributions can be neglected. Since $f_{1}^{q} \gg h_{1}^{\perp q}$ and $D_{1}^{q} \gg H_{1}^{\perp q}$, the suppression of the Cahn effect requires very large $Q^{2}$.

The SIDIS structure function $F_{U U}^{c o s 2 \phi_{h}}$ has already been measured by the CLAS Collaboration at JLab [500], the HERMES Collaboration at DESY [501], and the COMPASS Collaboration at CERN [502]. More precisely, typically data are shown for the relevant azimuthal asymmetry given by $F_{U U}^{\cos 2 \phi_{h}} / F_{U U}$. However, due to the limited range in $Q^{2}$ the present SIDIS data allow at most a qualitative extraction of $h_{1}^{\perp}$, as is also obvious from
a first exploratory study [367]. Moreover, the Boer-Mulders function for antiquarks is not at all constrained by the available data from SIDIS. Some information about antiquarks is available from recent Fermilab data on proton-deuteron [348] and proton-proton 349 DrellYan, though the uncertainties are again significant and not the least due to the presently large uncertainties for the Boer-Mulders function of quarks [370, 503, 504].

Even without further detailed reasoning it is clear that a quantitative knowledge about the Boer-Mulders function can only be obtained with data from new facilities. Measurements of the structure function $F_{U U}^{\cos 2 \phi_{h}}$ in the valence region in electroproduction of pions and kaons compose an important part of the upgraded JLab program on TMD studies. However, the $Q^{2}$ range obtainable with JLab12 will not be sufficient to suppress the contribution from the Cahn effect.

Only the unprecedented wide kinematic range of the EIC would provide clean measurements of the Boer-Mulders function for valence and sea quarks, and will allow for studying both, its $Q^{2}$ evolution and transition behavior from low to high $P_{h T}$.

Finally, there also exists a Boer-Mulders function for gluons, $h_{1}^{\perp g}$, describing the distribution of linearly polarized gluons in an unpolarized hadron [248, 281, 282]. In contrast to the Boer-Mulders function for quarks, $h_{1}^{\perp g}$ is T-even. See the relevant discussions in Sec. 3.

### 2.6 Overview on other TMDs

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In previous Sections, we discussed the unpolarized TMD $f_{1}$, the Sivers distribution $f_{1 T}^{\perp}$, the transversity distribution $h_{1}$, and the Boer-Mulders distribution $h_{1}^{\perp}$. They have been given more emphasis because at the present state of our knowledge they seem to be the most attractive and promising for EIC studies.

Nevertheless, interesting physics is embodied also in all other TMDs. Only the combination of information from all TMDs will fully explore the information contained in the unintegrated quark correlator, and provide a complete picture of the parton structure of the nucleon in transverse momentum space. This wealth of information may become one of the biggest legacies of the EIC.

In this Section, we briefly discuss the leading-twist TMDs that have not been analyzed in previous Sections and some of the sub-leading twist TMDs.

(a)
quark pol.

|  |  | U | L | T |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
|  | U | $f^{\perp}$ | $g^{\perp}$ | $\boldsymbol{e}$ | $h$ |
|  | L | $f_{L}^{\perp}$ | $g_{L}^{\perp}$ | $h_{L}$ | $e_{L}$ |
|  | T | $f_{T}, f_{T}^{\perp}$ | $\mathrm{g}_{T}, g_{T}^{\perp}$ | $h_{T}, h_{T}^{\perp}$ | $e_{T}, e_{T}^{\perp}$ |

(b)

Table 2.5. Transverse momentum dependent (a) twist-2, (b) twist-3 distribution functions. The $\mathrm{U}, \mathrm{L}, \mathrm{T}$ correspond to unpolarized, longitudinally polarized and transversely polarized nucleons (rows) and quarks (columns). Functions in boldface survive transverse momentum integration. Functions in gray cells are T-odd.

### 2.6.1 Other leading-twist TMDs

Table 2.5a summarizes the full list of leading-twist TMDs. The helicity distribution $g_{1}$, together with $f_{1}$ and $h_{1}$, survives integration over transverse momentum and has been already discussed extensively. Here we mention the importance of also studying its transverse momentum dependence. It may be possible that the transverse momentum distribution of quarks with spin antiparallel to the nucleon is different from that of quarks with spin parallel to the nucleon as suggested by lattice calculations [280] shown in Fig. [2.29] The structure function $F_{L L}$, involving the transverse-momentum dependence of $g_{1}$, is the only one where transverse-momentum resummation studies have been carried out to a level similar to $F_{U U, T}$ [372, but no extraction of the nonperturbative component has ever been attempted. The EIC will be an ideal machine to address this question.

The chiral-odd T-even TMD $h_{1 T}^{\perp}$ appears in the SIDIS structure function $F_{U T}^{\sin \left(3 \phi-\phi_{S}\right)}$. This function may be interpreted as the distribution of quarks with a polarization transverse but orthogonal to that of a transversely polarized nucleon. The popular name "pretzelosity" is due to the fact that this distribution has a quadrupole shape, vaguely reminiscent of a


Figure 2.29. Ratio between the helicity distribution and the unpolarized distribution for up quarks based on lattice QCD computations [280]: the significant $k_{\perp}$ dependence of the two curves (corresponding to two different parameterizations) suggests that quarks with different spin orientation have different transverse momentum distributions.
pretzel 411, 301. This TMD has attracted a lot of interest in the literature recently because of its possible connection with orbital angular momentum (see detailed discussion in Sec. (2.4.4). It is also interesting that, in a number of nonperturbative models, $h_{1 T}^{\perp}$ is just the difference between the quark helicity and the transversity distribution [419. Moreover, in simple spectator models of the nucleon it can be related to a particular linear combination of chiral-odd generalized parton distributions [282]. In general, $h_{1 T}^{\perp}$ involves an interference between light-cone wave function components that differ by two units of orbital angular momentum. Preliminary data from COMPASS [505] and from HERMES [506] taken with transversely polarized deuterons or protons, respectively, showed an effect compatible with zero, however, within large experimental uncertainties.

The TMDs $g_{1 T}$ and $h_{1 L}^{\perp}$ appear in the structure functions $F_{L T}^{\cos \left(\phi-\phi_{S}\right)}$ and $F_{U L}^{\sin 2 \phi}$, respectively. The chiral-even (chiral-odd) $g_{1 T}\left(h_{1 L}^{\perp}\right)$ describes longitudinally (transversely) polarized quarks in a transversely (longitudinally) polarized nucleon. Since both functions link two perpendicular spin directions, they are sometimes named "worm-gear" functions. Both functions are related to quark orbital motion inside nucleons. They represent the real part of an interference between nucleon wave functions that differ by one unit of orbital angular momentum, while the imaginary parts are related to the Sivers and Boer-Mulders functions [278, 507]. Because of this, they appear in positivity bounds together with the Sivers and Boer-Mulders function 507. They do not depend on final-state interactions and may offer cleaner insights into orbital angular momentum compared to the Sivers and Boer-Mulders functions. Interestingly, these functions are the first TMDs that have been computed on the lattice [279, 280]. The results (with the due caveats) indicate that they are sizable, $g_{1 T}^{u_{v}}>0, g_{1 T}^{d_{v}}<0$, and $g_{1 T} \approx-h_{1 L}^{\perp}$. These general findings also agree with some model calculations, see Sec. 2.4.4,

Notice that due to their chirality properties, $g_{1 T}$ couples through evolution to its analogous function for gluons (named $\Delta G_{T}$ in Ref. [281] and $g_{1 T}^{g}$ in Ref. [282]), while this is not true for $h_{1 L}^{\perp}$. This difference will be particularly relevant at the EIC, where gluons will play an important role.

By exploring QCD equations of motion, and neglecting "pure twist-3" quark-gluon correlators and current quark mass terms, one can express $g_{1 T}\left(h_{1 L}^{\perp}\right)$ in terms of $g_{1}\left(h_{1}\right)$ (see, e.g., [243, 252, 427, 508] and references therein). This is similar in spirit to the clas-
sic Wandzura-Wilczek approximation 509] for the twist-3 distribution function $g_{T}^{q}(x) \approx$ $\int_{x}^{1} \mathrm{~d} y g_{1}^{q}(y) / y$, (which is supported by the instanton QCD vacuum model [510, 511] and lattice QCD [512, 513]). At an initial stage, it may be convenient to exploit such Wandzura-Wilczek-type approximations, in order to make estimates for planned experiments [252, 508, 514]. In fact, existing data suggest that they are reasonable [508], even though at present there are no compelling grounds for supporting their validity [515, 516, 517]. In the end, these approximations should be tested and twist-3 effects should be extracted from the data, as we will also argue in the next subsection.

### 2.6.2 Subleading-twist TMDs

Eight out of the 18 structure functions providing the complete description of the SIDIS cross section are leading twist and were discussed in detail in previous sections. However, 10 structure functions are higher twist, where the underlying twist-classification follows [245]: "an observable is twist- $t$ if its effect is effectively suppressed by $(M / Q)^{t-2}$."

Higher twist functions, see Table [2.5b for a full list of twist-3 TMDs, are of interest for several reasons. Their understanding is required not only to complete the description of the SIDIS process. Besides being indispensable to correctly extract twist-2 parts from data, the knowledge of higher twists will also offer important tools to access the physics of the largely unexplored quark-gluon correlations which provide direct and unique insights into the dynamics inside hadrons, see, e.g., [518]. The EIC, which will span a large $Q$-range, will be an ideal tool to identify higher-twist effects, which fall off as powers of $1 / Q$.

Although suppressed with respect to twist-2 observables by $1 / Q$, twist- 3 observables are not small in the kinematics of fixed target experiments. Indeed, the first unambiguously measured single spin phenomena in SIDIS which triggered important theoretical developments, were the sizable longitudinal target $\left(A_{U L}^{\sin \phi}\right)$ and beam $\left(A_{L U}^{\sin \phi}\right)$ spin asymmetries observed at HERMES and JLab [519, 520, 521, 522, 523, 524]. Further data on twist-3 spin asymmetries are underway [505, 525, 526]. In unpolarized SIDIS, the sizable twist-3 effects $\left(A_{U U}^{\cos \phi}\right)$ are known since EMC [527, 528], see also recent results from JLab, HERMES and COMPASS [501, 529, 500, 530]. At high energies $A_{U U}^{\text {cos } \phi}$ can be described in perturbative QCD, and the unique possibilities of EIC could bridge [371 the gap to high energy data [531, 532, 533, 534. The understanding of the "matching" of the TMD formalism and the large- $p_{T}$ collinear description is of fundamental importance, see Sec. 2.2.5 and references therein.

The theoretical description of twist-3 observables is challenging. A good illustration of this point is that in spite of the enormous dedicated theoretical and phenomenological effort [396, 397, 465, 535, 536, 537, 538, 539, 540, 541, 542, 543, (544, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555, to explain the first single spin phenomena in SIDIS, $A_{U L}^{\sin \phi}$ and $A_{L U}^{\sin \phi}$, these observables are still not understood. The theoretical challenge is that presently it is not understood how to control light-cone divergences in SIDIS at $1 / Q$ order [555]. This does not necessarily mean there is no factorization, but it indicates that possibly new techniques are needed to pave the way towards a factorization proof in SIDIS at twist-3. If one assumes twist-3 TMD factorization, the phenomenological challenge is that each twist-3 observable receives contributions from several unknown twist-3 TMDs or fragmentation functions [247]. The situation simplifies in semi-inclusive jet production, a promising process to study at EIC energies, which could provide valuable complementary information on twist-3 TMDs [556].

An important process which can provide independent information on twist-3 (and, of course, also twist-2) TMDs are interference functions [451, 478, 479, 480, 476, [557, 558]. The advantage of this approach is that here collinear factorization applies, i.e. one cannot access TMDs. However, those functions which "survive" the $k_{\perp}$-integration of the quark correlator can be studied, and this includes at the twist- $3 e^{a}(x), g_{T}^{a}(x), h_{L}^{a}(x)$. These functions contribute to observables in convolution with specific interference fragmentation functions, which can be inferred from azimuthal asymmetries in $e^{+} e^{-}$annihilations 485].

There is no doubt that experimental, phenomenological and theoretical efforts to go beyond twist-2 are worth. Twist-3 functions describe multiparton distributions corresponding to the interference of higher Fock components in the hadron wave functions, and as such have no probabilistic partonic interpretations. Yet they offer fascinating insights into the nucleon structure [559. The Mellin moment $\int \mathrm{d} x x^{2} \tilde{g}_{T}^{a}(x)$ of the pure twist-3 piece in $g_{T}^{a}$ describes the transverse impulse the active quark acquires after being struck by the virtual photon due to the color Lorentz force. The Mellin moment $\int \mathrm{d} x x^{2} \tilde{e}^{a}(x)$ of the pure twist- 3 piece in $e^{a}(x)$ describes the average transverse force acting on a transversely polarized quark in an unpolarized target after interaction with the virtual photon.

Twist-3 TMDs are closely related to projections of different combinations of the collinear twist-3 correlation functions $G_{F}(x, x \prime)$ and $\tilde{G}_{F}(x, x \prime)$ discussed in Sec. [2.2.4, which are involved in the evolution equations of twist-3 collinear PDFs [560, 561, 562, 563, 564, 565, 566, and play important roles also in derivations of the evolution equations for transverse moments of TMDs [290, 291, 390, 391, 392, calculations of processes at high transverse momentum [352, or calculations of the high transverse momentum tails of TMDs [292, 295]. Ultimately, through a global study of all of these observables, one could simultaneously obtain better knowledge of twist-3 collinear functions and twist-2 TMDs, and at the same time test the validity of the formalism. Gathering as much information as one can on the quark-gluon-quark correlator is essential to reach this goal.

## Chapter 3

# Three-dimensional structure of the proton and nuclei: spatial imaging 

Convenors and chapter editors:
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### 3.1 Spatial imaging of sea quarks and gluons: summary

V. Guzey, F. Sabatié, M. Burkardt

The internal landscape of the nucleon and nuclei in terms of the fundamental quarks and gluons can be studied in different hard processes and can be characterized by different quantities (distributions). Hard exclusive reactions such as deeply virtual Compton scattering (DVCS) and exclusive production of mesons give an access to the aspects of the hadron structure that are encoded in generalized parton distributions (GPDs) and dipole amplitudes.

GPDs generalize the well-known form factors, distribution amplitudes and parton distributions and quantify various correlations/distributions of quarks and gluons in terms of their momentum fractions and positions in the transverse plane. Thus, GPDs provide a rigorous framework for studies of the three-dimensional parton structure of hadrons as well as many additional important aspects of the hadron structure such as the parton angular momentum and the related "spin puzzle", spin and flavor content, the role of chiral symmetry, and many more.

At the moment, our knowledge about GPDs is mostly limited to valence quark GPDs (Hermes, Compass, Jefferson Lab 6 GeV and also Jefferson Lab 12 GeV in the near future) and rather low precision data from HERA. A high-energy high-luminosity Electron-Ion Collider (EIC) will be an ideal machine for the studies of hard exclusive reactions and sea quark and gluon GPDs as summarised in table 3.1.
\(\left.$$
\begin{array}{|c|c|c|c|}\hline \text { Deliverables } & \text { Observables } & \text { What we learn } & \text { Requirements } \\
\hline \hline \text { sea quark and } & \text { DVCS and } J / \psi, \rho, \phi \\
\text { gluon GPDs } \\
\text { production cross sect. } \\
\text { and asymmetries }\end{array}
$$ $$
\begin{array}{c}\text { transverse images of } \\
\text { sea quarks and gluons } \\
\text { in nucleon and nuclei; } \\
\text { total angular momentum; } \\
\text { onset of saturation }\end{array}
$$ \quad \begin{array}{c}\mathcal{L} \geq 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}, <br>
Roman Pots <br>
wide range of x_{B} and Q^{2} <br>
polarized e^{-} and p beams <br>

e^{+} beam for DVCS\end{array}\right]\)| $\mathcal{L} \geq 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ |
| :---: |
| quark GPDs |

Table 3.1. Science Matrix for Exclusive Processes at EIC.
(i) One essential aspect of the GPD program is obtaining the transverse image of quarks and gluons in the nucleon/nucleus through the measurement of the $t$ dependence of cross sections of various exclusive processes (DVCS, production of $J / \psi, \phi, \pi, K$, etc. mesons) in a wide range of $t$. In the nucleon case, covering the interval $0 \approx|t| \leq 2 \mathrm{GeV}^{2}$ will enable one to map out the parton distributions in the transverse plane of the impact parameter $b$ down to as low as $b \approx 0.1 \mathrm{fm}$.
(ii) One area where an EIC shines is the large range in $Q^{2}$ available in the full $x_{B}$ interval. QCD evolution equations of GPDs, similarly to the PDF case, allow one to globally fit the data using flexible parameterizations of GPDs and to extract accurate and model-
independent information on GPDs. One also will use the large lever arm in $Q^{2}$ to establish the reaction mechanisms (scaling properties, higher twist effects).
(iii) Another clear advantage of an EIC is the availability of different polarizations for the lepton and proton beams that allows one to fully disentangle the various GPDs from the experimental observables. While DVCS is sensitive to singlet quark and gluon GPDs, other exclusive diffractive processes (electroproduction of $\rho, J / \psi, \phi$, etc.) and non-diffractive processes (electroproduction of $\pi^{+}, K^{+}$, etc.) will allow one to access the spin and flavor dependences of GPDs. Note that the non-diffractive processes push the requirements for high luminosity much further than DVCS or other diffractive processes.
(iv) Exclusive processes with nuclei in a collider and, subsequently, the spatial image of sea quarks and gluons in nuclei will be studied for the first time. All the processes mentioned above will benefit from the high luminosity of an EIC (of the order of $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ ) as well as excellent detection capabilities and particle identification guaranteeing exclusivity.
The contributions below describe in detail various aspects of the rich program of spatial imaging of sea quarks and gluons at an EIC. In conclusion, a high-energy high-luminosity EIC, studying various deep exclusive processes through cross sections and polarization observables, would uniquely extend and complement our knowledge of the 3D partonic structure of the nucleon/nucleus to the sea of quarks and gluons.

### 3.2 Basics of generalized parton distributions

Anatoly Radyushkin

### 3.2.1 Introduction

The fundamental physics to be accessed via the generalized parton distributions (GPDs) [274, 567, 568, 569, 570, 571, 572] is the structure of hadrons. This is a rather general statement, and we may want to have a more specific one. A classic example of such a specific case is the search for the Higgs boson (HB) performed currently at the Large Hadron Collider (LHC). The motivation for the search is that HB is supposed to be responsible for generation of masses, in particular, quark masses. However, by far, the largest part of visible mass is due to the nucleons, and out of 940 MeV of the nucleon mass, less than 30 MeV (current quark masses) may be related to HB. The remaining $97 \%$ of the nucleon mass is due to gluons - which are massless! This is a characteristic illustration of the situation in hadron physics:
i) All the relevant particles are already established, i.e., no "higgses" to find.
ii) The QCD Lagrangian is known.
iii) However, we still need to understand how QCD works, i.e., to understand hadronic structure in terms of quark and gluon fields.

Projecting quark and gluon fields $q\left(z_{1}\right), q\left(z_{2}\right), \ldots$ onto hadronic states $|p, s\rangle$ gives matrix elements:

$$
\begin{equation*}
\langle 0| \bar{q}_{\alpha}\left(z_{1}\right) q_{\beta}\left(z_{2}\right)|M(p), s\rangle \quad, \quad\langle 0| q_{\alpha}\left(z_{1}\right) q_{\beta}\left(z_{2}\right) q_{\gamma}\left(z_{3}\right)|B(p), s\rangle \tag{3.1}
\end{equation*}
$$

that can be interpreted as hadronic wave functions. In particular, in the light-cone (LC) formalism [573], a hadron is described by its Fock components in the infinite-momentum frame. For the nucleon, one can schematically write:

$$
\begin{equation*}
|P\rangle=\Psi_{q q q}\left|q\left(x_{1} P, k_{1 \perp}\right) q\left(x_{2} P, k_{2 \perp}\right) q\left(x_{3} P, k_{3 \perp}\right)\right\rangle+\Psi_{q q q G}|q q q G\rangle+\Psi_{q q q \bar{q} q}|q q q \bar{q} q\rangle+\ldots, \tag{3.2}
\end{equation*}
$$

where $x_{i}$ are momentum fractions satisfying $\sum_{i} x_{i}=1 ; k_{i \perp}$ are transverse momenta, $\sum_{i} k_{i \perp}=0 ; \Psi$ are light-cone wave functions. In principle, solving the bound-state equation $H|P\rangle=E|P\rangle$ one should get the wave function $|P\rangle$ that contains complete information about the hadron structure. In practice, however, the equation (involving an infinite number of Fock components) has not been solved yet in the realistic 4-dimensional case. Moreover, the LC wave functions are not directly accessible experimentally.

The way out of this situation is the description of hadron structure in terms of phenomenological functions. Among the "old" functions used for a long time we can list form factors, usual parton densities, and distribution amplitudes. The "new" functions, generalized parton distributions (for reviews, see [574, 575, 576, [577]), are hybrids of form factors, parton densities and distribution amplitudes. Furthermore, the "old" functions are limiting cases of the "new" ones.

### 3.2.2 Form factors

The form factors are defined through matrix elements of electromagnetic (EM) and weak currents between hadronic states. In particular, the nucleon electromagnetic form factors are given by

$$
\begin{equation*}
\left\langle p^{\prime}, s^{\prime}\right| J^{\mu}(0)|p, s\rangle=\bar{u}\left(p^{\prime}, s^{\prime}\right)\left[\gamma^{\mu} F_{1}(t)+\frac{r^{\nu} \sigma^{\mu \nu}}{2 m_{N}} F_{2}(t)\right] u(p, s), \tag{3.3}
\end{equation*}
$$

where $r=p-p^{\prime}$ is the momentum transfer and $t=r^{2}$. The electromagnetic current is given by the sum of its flavor components:

$$
\begin{equation*}
J^{\mu}(z)=\sum_{f} e_{f} \bar{\psi}_{f}(z) \gamma^{\mu} \psi_{f}(z) \tag{3.4}
\end{equation*}
$$

The nucleon helicity non-flip form factor $F_{1}(t)$ can also be written as a sum $\sum_{f} e_{f} F_{1 f}(t)$. A similar decomposition holds for the helicity flip form factor $F_{2}(t)=\sum_{f} e_{f} F_{2 f}(t)$. At $t=0$, these functions have well known limiting values. In particular, $F_{1}(t=0)=e_{N}=\sum_{f} N_{f} e_{f}$ gives total electric charge of the nucleon ( $N_{f}$ is the number of valence quarks of flavor $f$ ) and $F_{2}(t=0)=\kappa_{N}$ gives its anomalous magnetic moment. The form factors are measurable through elastic $e N$ scattering.


Figure 3.1. Elastic $e N$ scattering in the one-photon exchange approximation.

### 3.2.3 Usual parton densities

The parton densities are defined through forward matrix elements of quark/gluon fields separated by light-like distances. In particular, in the unpolarized case we have

$$
\begin{equation*}
\left.\langle p| \bar{\psi}_{a}(-z / 2) \gamma^{\mu} \psi_{a}(z / 2)|p\rangle\right|_{z^{2}=0}=2 p^{\mu} \int_{0}^{1}\left[e^{-i x(p z)} f_{a}(x)-e^{i x(p z)} f_{\bar{a}}(x)\right] d x \tag{3.5}
\end{equation*}
$$

In the local limit $z=0$, the operators in this definition coincide with the operators contributing into the non-flip form factor $F_{1}$. Since $t=0$ for the forward matrix element, we obtain the sum rule for the numbers of valence quarks:

$$
\begin{equation*}
\int_{0}^{1}\left[f_{a}(x)-f_{\bar{a}}(x)\right] d x=N_{a} . \tag{3.6}
\end{equation*}
$$

The definition of parton densities has the form of the plane wave decomposition. This observation allows one to give the momentum space interpretation: $f_{a(\bar{a})}(x)$ is the probability to find $a(\bar{a})$-quark with momentum $x p$ inside a nucleon with momentum $p$. The classic process to access the usual parton densities is deep inelastic scattering (DIS) $\gamma^{*} N \rightarrow X$.

Using the optical theorem, the $\gamma^{*} N \rightarrow X$ cross section is given by the imaginary part of the forward virtual Compton scattering amplitude. The momentum transfer $q$ is spacelike $q^{2} \equiv-Q^{2}$, and when it is sufficiently large, perturbative QCD factorization works. At the leading order, one deals with the so-called handbag diagram, see figure 3.2.

Through simple algebra, $\frac{1}{\pi} \operatorname{Im} 1 /(q+x p)^{2} \approx \delta\left(x-x_{B}\right) / 2(p q)$, one finds that DIS measures parton densities at the point $x=x_{B}$, where the parton momentum fraction equals the Bjorken variable $x_{B}=Q^{2} / 2(p q)$. Comparing parton densities to form factors, we note that the latter have a point vertex instead of a light-like separation and $p \neq p^{\prime}$.


Figure 3.2. Lowest order pQCD factorization for DIS.

### 3.2.4 Nonforward parton densities

"Hybridization" of different parton distributions is the key idea of the GPD approach. As the first step, we can combine form factors with parton densities [578] and write the flavor components $F_{1 a}(t)$ of form factors as integrals over the momentum fraction variable $x$ :

$$
\begin{equation*}
F_{1 a}(t)=\int_{0}^{1}\left[\mathcal{F}_{a}(x, t)-\mathcal{F}_{\bar{a}}(x, t)\right] d x . \tag{3.7}
\end{equation*}
$$

In the forward limit $t=0$, the new objects-nonforward parton densities $\mathcal{F}_{a(\bar{a})}(x, t)$ (NPDs) - coincide with the usual ("forward") densities:

$$
\begin{equation*}
\mathcal{F}_{a(\bar{a})}(x, t=0)=f_{a(\bar{a})}(x) . \tag{3.8}
\end{equation*}
$$

NPDs can be also treated as Fourier transforms of the impact parameter $b_{\perp}$ distributions $f\left(x, b_{\perp}\right)$ describing the variation of parton densities in the transverse plane [579, 580].

A nontrivial question is the interplay between $x$ and $t$ dependencies of $\mathcal{F}_{a(\bar{a})}(x, t)$. The simplest factorized ansatz $\mathcal{F}_{a}(x, t)=f_{a}(x) F_{1}(t)$ satisfies both the forward constraint, $\mathcal{F}_{a}(x, t=0)=f_{a}(x)$, and also the local constraint (3.7). The reality may be more complicated: light-cone wave functions with Gaussian $k_{\perp}$ dependence

$$
\begin{equation*}
\Psi\left(x_{i}, k_{i \perp}\right) \sim \exp \left[-\frac{1}{\lambda^{2}} \sum_{i} k_{i \perp}^{2} / x_{i}\right] \tag{3.9}
\end{equation*}
$$

suggest that

$$
\begin{equation*}
\mathcal{F}^{a}(x, t)=f_{a}(x) e^{\bar{x} t / 2 x \lambda^{2}} \tag{3.10}
\end{equation*}
$$

where $\bar{x} \equiv 1-x$. Taking $f_{a}(x)$ from existing parametrizations and adjusting $\lambda^{2}$ to provide the standard value of the quark intrinsic transverse momentum $\left\langle k_{\perp}^{2}\right\rangle \approx(300 \mathrm{MeV})^{2}$ gives a rather reasonable description of the proton form factor $F_{1}(t)$ in a wide range of momentum transfers $-t \sim 1-10 \mathrm{GeV}^{2}$ [578]. To comply with the Regge behavior, one may wish to change $e^{\bar{x} t / 2 x \lambda^{2}} \rightarrow x^{-\alpha^{\prime} t}$, where $\alpha^{\prime}$ is the Regge trajectory slope. The modified Regge ansatz,

$$
\begin{equation*}
\mathcal{F}^{a}(x, t)=f_{a}(x) x^{-\alpha^{\prime}(1-x) t} \tag{3.11}
\end{equation*}
$$

allows one to easily fit electromagnetic form factors for the proton and neutron 581]. A similar model was proposed in Ref. 582].

The same nonforward parton densities appear in the handbag diagrams for the wideangle real Compton scattering, see figure 3.3.


Figure 3.3. Form factor and wide-angle Compton scattering amplitude in terms of nonforward parton densities.

The handbag contribution is approximately given by the product of a new form factor, $R_{V}^{a}(t)$, and the cross section of the Compton scattering off an elementary fermion (given by Klein-Nishina expression):

$$
\begin{equation*}
\frac{d \sigma}{d t}=\left.\left[\sum_{a} e_{a}^{2} R_{V}^{a}(t)\right]^{2} \frac{d \sigma}{d t}\right|_{K N} \quad \text { with } \quad R_{V}^{a}(t)=\int_{0}^{1} \frac{\mathcal{F}^{a}(x, t)}{x} d x \tag{3.12}
\end{equation*}
$$

The predictions based on handbag dominance and NPDs [578, 583] are in much better agreement with the existing data [584] than the predictions based on two-gluon hard exchange mechanism of asymptotic perturbative QCD: the predicted cross section is too small in the latter case. The absolute normalization for predictions is settled by the form of the nonperturbative functions (NPDs in the handbag approach and nucleon distribution amplitudes in the pQCD approach) which were fixed by fitting the $F_{1}$ form factor data. Still, when there is an uncertain overall factor, it is risky to make strong statements. Remarkably, the perturbative QCD hard scattering mechanism and soft handbag mechanism give drastically different predictions for the polarization asymmetry $A_{L L}$ [583. Experiment E-99-114 performed at Jefferson Lab 584 strongly favors handbag mechanism that predicts the value close to the asymmetry for the scattering on a single quark.

### 3.2.5 Distribution amplitudes

Another example of nonperturbative functions describing the hadron structure are the distribution amplitudes (DAs). They can be interpreted as light cone wave functions integrated over transverse momentum, or as $\langle 0| \ldots|p\rangle$ matrix elements of light cone operators. In the case of the pion, we have

$$
\begin{equation*}
\left.\langle 0| \bar{\psi}_{d}(-z / 2) \gamma_{5} \gamma^{\mu} \psi_{u}(z / 2)\left|\pi^{+}(p)\right\rangle\right|_{z^{2}=0}=i p^{\mu} f_{\pi} \int_{-1}^{1} e^{-i \alpha(p z) / 2} \varphi_{\pi}(\alpha) d \alpha \tag{3.13}
\end{equation*}
$$

with $x_{1}=(1+\alpha) / 2, x_{2}=(1-\alpha) / 2$ being the fractions of the pion momentum carried by the quarks. The distribution amplitudes describe the hadrons in situations when the pQCD hard scattering approach is applicable to exclusive processes. The classic example is the $\gamma^{*} \gamma \rightarrow \pi^{0}$ transition; its amplitude is proportional to the $1 /\left(1-\alpha^{2}\right)$ moment of $\varphi_{\pi}(\alpha)$, see figure 3.4, left. The predictions for the $\gamma^{*} \gamma \rightarrow \pi^{0}$ form factor based on two competing models for the pion DA, the asymptotic $\varphi_{\pi}^{\text {as }}(\alpha)=\frac{3}{4}\left(1-\alpha^{2}\right)$ and Chernyak-Zhitnitsky DA $\varphi_{\pi}^{\mathrm{CZ}}(\alpha)=\frac{15}{4} \alpha^{2}\left(1-\alpha^{2}\right)$ differ by factor of $5 / 3$, and the hope was that this difference would allow for an experimental discrimination between them. Indeed, the comparison with CLEO and CELLO data for $Q^{2} F_{\gamma^{*} \gamma \pi^{0}}\left(Q^{2}\right)$ that extend to $Q^{2} \lesssim 10 \mathrm{GeV}^{2}$ favors DAs that are closer
to $\varphi^{\text {as }}(\alpha)$. However, recent BABAR data covering the range up to $Q^{2} \sim 40 \mathrm{GeV}^{2}$ show the increase of $Q^{2} F_{\gamma^{*} \gamma \pi^{0}}\left(Q^{2}\right)$ for $Q^{2} \gtrsim 10 \mathrm{GeV}^{2}$. To explain this increase, the scenarios were proposed in which the pion DA does not vanish at the end-points, e.g., $\varphi_{\pi}^{\text {flat }}(\alpha)=1$.


Figure 3.4. Lowest-order pQCD factorization for $\gamma^{*} \gamma \rightarrow \pi^{0}$ transition amplitude and for the pion electromagnetic form factor.

Another classic application of pQCD to exclusive processes is the pion electromagnetic form factor, see figure 3.4, right. With the asymptotic pion DA $\varphi_{\pi}^{\text {as }}(\alpha)$, the hard pQCD contribution to $F_{\pi}\left(Q^{2}\right)$ is $\left(2 \alpha_{s} / \pi\right)\left(0.7 \mathrm{GeV}^{2}\right) / Q^{2}$, which is less than $1 / 3$ of the experimental value. Taking wider DAs formally increases the size of the one-gluon-exchange contribution, but it is dominated then by the regions where the gluon virtuality is too small to be treated perturbatively. So, in this case we deal with the dominance of the competing soft mechanism which is described by nonforward parton densities, exactly in the same way as the proton form factor $F_{1}^{p}(t)$ discussed in the previous section.

### 3.2.6 Hard electroproduction processes

An attempt to use perturbative QCD to extract new information about hadronic structure is the study of deep exclusive photon [274] or meson [569, [572] electroproduction reactions. In the hard kinematics when both $Q^{2}$ and $s \equiv(p+q)^{2}$ are large while the momentum transfer $t \equiv\left(p-p^{\prime}\right)^{2}$ is small, one can use pQCD factorization which represents the amplitudes as a convolution of a perturbatively calculable short-distance amplitude and nonperturbative parton functions describing the hadron structure. The hard pQCD subprocesses in these two cases have different structure, see figure 3.5. Since the photon is a pointlike particle, the deeply virtual Compton scattering (DVCS) amplitude has the structure similar to that of the $\gamma^{*} \gamma \pi^{0}$ form factor: the pQCD hard term is of zero order in $\alpha_{s}$ (the handbag mechanism), and there is no competing soft contribution. Thus, we can expect that pQCD works from $Q^{2} \sim 2 \mathrm{GeV}^{2}$. On the other hand, the deeply virtual meson production process is similar to the pion EM form factor: the hard term has a $O\left(\alpha_{s} / \pi\right) \sim 0.1$ suppression factor. As a result, the dominance of the hard pQCD term may be postponed to $Q^{2} \sim 5-10 \mathrm{GeV}^{2}$.


Figure 3.5. Lowest-order factorization for deeply virtual photon and meson production.

One should also have in mind that the competing soft mechanism can mimic the same power-law $Q^{2}$-behavior (just like in case of pion and nucleon EM form factors). Hence, a mere observation of a "right" power-law behavior of the cross section may be insufficient to claim that pQCD is already working. One should look at other characteristics of the reaction, especially its spin properties, to make strong statements about the reaction mechanism.

### 3.2.7 Deeply virtual Compton scattering and generalized parton distributions

It is convenient to visualize DVCS in the $\gamma^{*} N$ center-of-mass frame, with the initial hadron and the virtual photon moving in opposite directions along the $z$-axis. Since the momentum transfer $t$ is small, the hadron and the real photon in the final state also move close to the $z$-axis. This means that the virtual photon momentum $q=q^{\prime}-x_{B} p$ has the component $-x_{B} p$ canceled by the momentum transfer $r$. In other words, the momentum transfer $r$ has the longitudinal component $r^{+}=x_{B} p^{+}$, where $x_{B}=Q^{2} / 2(p q)$ is the DIS Bjorken variable. One can say that DVCS has a skewed kinematics in which the final hadron has the "plus" momentum $(1-\zeta) p^{+}$that is smaller than that of the initial hadron. In the particular case of DVCS, we have $\zeta=x_{B}$.

The parton picture for DVCS has some similarity to that of DIS, with the main difference that the plus-momenta of the incoming and outgoing quarks in DVCS are not equal; they are $X p^{+}$and $(X-\zeta) p^{+}$, see figure 3.6. Another difference is that the invariant momentum transfer $t$ in DVCS is nonzero: the matrix element of partonic fields is essentially nonforward.

Thus, the nonforward parton distributions (NFPDs) $\mathcal{F}_{\zeta}(X, t)$ describing the hadronic structure in DVCS depend on $X$ (the fraction of $p^{+}$carried by the outgoing quark), $\zeta$ (the skewness parameter characterizing the difference between initial and final hadron momenta), and $t$ (the invariant momentum transfer). In the forward $r=0$ limit, we have a reduction formula

$$
\begin{equation*}
\mathcal{F}_{\zeta=0}^{a}(X, t=0)=f_{a}(X) \tag{3.14}
\end{equation*}
$$

relating NFPDs with the usual parton densities. The nontriviality of this relation is that $\mathcal{F}_{\zeta}(X, t)$ appear in the amplitude of the exclusive DVCS process, while the usual parton densities are measured from the cross section of the inclusive DIS reaction.

Another limit for NFPDs is zero skewness $\zeta=0$, where they correspond to nonforward parton densities: $\mathcal{F}_{\zeta=0}^{a}(X, t)=\mathcal{F}^{a}(X, t)$. The local limit relates NFPDs to form factors:

$$
\begin{equation*}
\int_{0}^{1} \mathcal{F}_{\zeta}^{a}(X, t) \frac{d X}{1-\zeta / 2}=F_{1}^{a}(t) \tag{3.15}
\end{equation*}
$$

The description in terms of NFPDs has the advantage of using the variables most close to those of the usual parton densities. However, the initial and final hadron momenta are not treated symmetrically in this scheme. Ji [274] proposed to use symmetric variables in which the plus-momenta of the hadrons are $(1+\xi) P^{+}$and $(1-\xi) P^{+}$, and those of the active partons are $(x+\xi) P^{+}$and $(x-\xi) P^{+}, P$ being the average momentum $P=\left(p+p^{\prime}\right) / 2$, see figure 3.6. In the simplified case of scalar fields, the GPD parametrization of the nonforward matrix element is

$$
\begin{equation*}
\langle P+r / 2| \psi(-z / 2) \psi(z / 2)|P-r / 2\rangle=\int_{-1}^{1} e^{-i x(P z)} H(x, \xi) d x+\mathcal{O}\left(z^{2}\right) . \tag{3.16}
\end{equation*}
$$



Figure 3.6. Comparison of NFPDs and OFPDs.

To take into account the spin properties of hadrons and quarks, one needs four offforward parton distributions $H, E, \tilde{H}, \widetilde{E}$, each of which is a function of $x, \xi$, and $t$. The skewness parameter $\xi \equiv r^{+} / 2 P^{+}$can be expressed in terms of the Bjorken variable, $\xi=$ $x_{B} /\left(2-x_{B}\right)$, but it does not coincide with it.

Depending on the value of $x$, each GPD has 3 distinct regions. When $\xi<x<1$, GPDs are analogous to usual quark distributions; when $-1<x<-\xi$, they are similar to antiquark distributions. In the region $-\xi<x<\xi$, the "returning" quark has a negative momentum and should be treated as an outgoing antiquark with momentum $(\xi-x) P$. The total $q \bar{q}$ pair momentum $r=2 \xi P$ is shared by the quarks in fractions $r(1+x / \xi) / 2$ and $r(1-x / \xi) / 2$. Hence, a GPD in the region $-\xi<x<\xi$ is similar to a distribution amplitude $\Phi(\alpha)$ with $\alpha=x / \xi$.

In the local limit, GPDs reduce to elastic form factors:

$$
\begin{equation*}
\sum_{a} e_{a} \int_{-1}^{1} H^{a}(x, \xi ; t) d x=F_{1}(t) \quad, \quad \sum_{a} e_{a} \int_{-1}^{1} E^{a}(x, \xi ; t) d x=F_{2}(t) \tag{3.17}
\end{equation*}
$$

The $E$ function, like $F_{2}(t)$, comes with the $r_{\mu}$ factor. Hence, it is invisible in DIS described by the forward $r=0$ Compton amplitude. However, the $t=0, \xi=0$ limit of $E$ exists:

$$
\begin{equation*}
E^{a, \bar{a}}(x, \xi=0 ; t=0) \equiv \kappa^{a, \bar{a}}(x) \tag{3.18}
\end{equation*}
$$

In particular, its integral gives the proton anomalous magnetic moment $\kappa_{p}$,

$$
\begin{equation*}
\sum_{a} e_{a} \int_{-0}^{1}\left(\kappa^{a}(x)-\kappa^{\bar{a}}(x)\right) d x=\kappa_{p} \tag{3.19}
\end{equation*}
$$

while its first moment enters Ji's sum rule for the total quark contribution $J_{q}$ to the proton spin:

$$
\begin{equation*}
J_{q}=\frac{1}{2} \sum_{a} \int_{-0}^{1} x\left[f^{a}(x)+f^{\bar{a}}(x)+\kappa^{a}(x)+\kappa^{\bar{a}}(x)\right] d x . \tag{3.20}
\end{equation*}
$$

Note that only valence quarks contribute to $\kappa_{p}$, while $J_{q}$ involves also sea quarks. Furthermore, the values of $\kappa_{p, n}$ (unlike $e_{p, n} \equiv F_{1}^{p, n}(0)$ ) strongly depend on dynamics, e.g., $\kappa_{N} \sim 1 / m_{q}$ in constituent quark models.

### 3.2.8 Double distributions

To model GPDs, two approaches are used: a direct calculation in specific dynamical models: bag model, chiral soliton model, light-cone formalism, etc., and a phenomenological construction based on the relation of GPDs to usual parton densities $f_{a}(x), \Delta f_{a}(x)$ and form factors $F_{1}(t), F_{2}(t), G_{A}(t), G_{P}(t)$. The key question in the second approach is the interplay between $x, \xi$ and $t$ dependencies of GPDs. There are not so many cases in which the pattern of the interplay is evident. One example is the function $\widetilde{E}(x, \xi, t)$ which is related to the $G_{P}(t)$ form factor and is dominated for small $t$ by the pion pole term $1 /\left(t-m_{\pi}^{2}\right)$. It is also proportional to the pion distribution amplitude $\varphi_{\pi}(\alpha)$ taken at $\alpha=x / \xi$. The construction of self-consistent models for other GPDs can be performed using an ansatz based on the formalism of double distributions (DD) [585].

The main idea behind the double distributions is a "superposition" of $P^{+}$and $r^{+}$momentum flows, i.e., the representation of the parton momentum $k^{+}=\beta P^{+}+(1+\alpha) r^{+} / 2$ as the sum of a component $\beta P^{+}$due to the average hadron momentum $P$ (flowing in the $s$-channel) and a component $(1+\alpha) r^{+} / 2$ due to the $t$-channel momentum $r$, see figure 3.7 , In the simplified case of scalar fields, the DD parametrization reads

$$
\begin{equation*}
\langle P-r / 2| \psi(-z / 2) \psi(z / 2)|P+r / 2\rangle=\int_{\Omega} F(\beta, \alpha) e^{-i \beta(P z)-i \alpha(r z) / 2} d \beta d \alpha+\mathcal{O}\left(z^{2}\right) . \tag{3.21}
\end{equation*}
$$

Thus, the double distribution $f(\beta, \alpha)$ (we consider here for simplicity the $t=0$ limit) looks like a usual parton density with respect to $\beta$ and like a distribution amplitude with respect to $\alpha$. The connection between the DD variables $\beta, \alpha$ and the GPD variables $x, \xi$ is obtained from $r^{+}=2 \xi P^{+}$, which results in the basic relation $x=\beta+\xi \alpha$. The formal connection between DDs and GPDs is

$$
\begin{equation*}
H(x, \xi)=\int_{\Omega} F(\beta, \alpha) \delta(x-\beta-\xi \alpha) d \beta d \alpha \tag{3.22}
\end{equation*}
$$



Figure 3.7. Comparison of GPD and DD descriptions.

The forward limit $\xi=0, t=0$ corresponds to $x=\beta$, and gives the relation between DDs and the usual parton densities:

$$
\begin{equation*}
\int_{-1+|\beta|}^{1-|\beta|} F_{a}(\beta, \alpha ; t=0) d \alpha=f_{a}(\beta) . \tag{3.23}
\end{equation*}
$$

The DDs live on the rhombus $|\alpha|+|\beta| \leq 1$ [denoted by $\Omega$ in (3.21) and (3.221)] and are symmetric functions of the "DA" variable $\alpha$ : $f_{a}(\beta, \alpha ; t)=f_{a}(\beta,-\alpha ; t)$ ("Munich" symmetry [586]). These restrictions suggest a factorized representation for a DD in the form of
a product of a usual parton density in the $\beta$-direction and a distribution amplitude in the $\alpha$-direction:

$$
\begin{equation*}
F(\beta, \alpha)=f(\beta) h(\beta, \alpha), h_{N}(\beta, \alpha) \sim \frac{\left[(1-|\beta|)^{2}-\alpha^{2}\right]^{N}}{(1-|\beta|)^{2 N+1}}, \int_{-1+|\beta|}^{1-|\beta|} h(\beta, \alpha) d \alpha=1 \tag{3.24}
\end{equation*}
$$

To obtain usual parton densities from DDs, one should integrate (scan) them over the vertical lines $\beta=x=$ const. To obtain the GPD $H(x, \xi)$ with nonzero $\xi$ from DDs $f(\beta, \alpha)$, one should integrate (scan) DDs along the parallel lines $\alpha=(x-\beta) / \xi$ with a $\xi$-dependent slope. One can call this process the DD-tomography. The basic feature of GPDs $H(x, \xi)$ resulting from DDs is that for $\xi=0$ they reduce to usual parton densities, and for $\xi=1$ they have a shape like a meson distribution amplitude. A more complete truth is that such a DD modeling misses terms invisible in the forward limit: meson-exchange contributions and so-called D-term, which can be interpreted as $\sigma$-exchange. The inclusion of the D-term induces nontrivial behavior in the central $|x|<\xi$ region (for details, see [587]).

### 3.2.9 GPDs and the structure of hadrons

Hadronic structure is a complicated subject, and it requires a study from many sides and in many different types of experiments. The description of specific aspects of hadronic structure is provided by several different functions: form factors, usual parton densities, distribution amplitudes. Generalized parton distributions provide a unified description: all these functions can be treated as particular or limiting cases of GPDs $H(x, \xi, t)$.

Usual parton densities $f(x)$ correspond to the case $\xi=0, t=0$. They describe a hadron in terms of probabilities $\sim|\Psi|^{2}$. However, QCD is a quantum theory: GPDs with $\xi \neq 0$ describe correlations $\sim \Psi_{1}^{*} \Psi_{2}$. Taking only the point $t=0$ corresponds to integration over impact parameters $b_{\perp}$ - information about the transverse structure is lost.

Form factors $F(t)$ contain information about the distribution of partons in the transverse plane, but $F(t)$ involve integration over momentum fraction $x$ - information about longitudinal structure is lost.

A simple "hybridization" of usual densities and form factors in terms of NPDs $\mathcal{F}(x, t)$ (GPDs with $\xi=0$ ) shows that the behavior of $F(t)$ is governed both by transverse and longitudinal distributions. GPDs provide adequate description of nonperturbative soft mechanism. They also allow to study transition from soft to hard mechanism.

Distribution amplitudes $\varphi(x)$ provide quantum-level information about the longitudinal structure of hadrons. In principle, they are accessible in exclusive processes at large momentum transfer, when hard scattering mechanism dominates. GPDs have DA-type structure in the central region $|x|<\xi$.

Generalized parton distributions $H(x, \xi, t)$ provide a 3 -dimensional picture of hadrons. GPDs also provide some novel possibilities, such as "magnetic distributions" related to the spin-flip GPD $E(x, \xi, t)$. In particular, the structure of nonforward density $E(x, \xi=0, t)$ determines the $t$-dependence of $F_{2}(t)$. Recent JLab data give $F_{2}(t) / F_{1}(t) \sim 1 / \sqrt{-t}$ rather than $1 / t$ expected in hard pQCD and many models - a puzzle waiting to be resolved. The forward reductions $\kappa^{a}(x)$ of $E(x, \xi, t)$ look as fundamental as $f^{a}(x)$ and $\Delta f^{a}(x)$ : Ji's sum rule involves $\kappa^{a}(x)$ on equal footing with $f(x)$. Magnetic properties of hadrons are strongly sensitive to dynamics providing a testing ground for models. Another novel possibility is the study of flavor-nondiagonal distributions, e.g., proton-to-neutron GPDs accessible through processes like exclusive charged pion electroproduction, proton-to- $\Lambda$ GPDs (they appear in kaon electroproduction), and proton-to- $\Delta$ GPDs - these can be related to form factors of
proton-to- $\Delta$ transition (another puzzle for hard pQCD). The GPDs for $N \rightarrow N+\operatorname{soft} \pi$ processes can be used for testing the soft pion theorems and physics of chiral symmetry breaking.

An interesting problem is the separation and flavor decomposition of GPDs. The DVCS amplitude involves all four types of GPDs, $H, E, \widetilde{H}, \widetilde{E}$, so we need to study other processes involving different combinations of GPDs. An important observation is that, in hard electroproduction of mesons, the spin nature of produced meson dictates the type of GPDs involved, e.g., for pion electroproduction, only $\widetilde{H}, \widetilde{E}$ appear, with $\widetilde{E}$ dominated by the pion pole at small $t$. This gives an access to (generalization of) polarized parton densities without polarizing the target.

In summary, the structure of hadrons is the fundamental physics to be accessed via GPDs. GPDs describe hadronic structure on the quark-gluon level and provide a threedimensional picture ("tomography") of the hadronic structure. GPDs adequately reflect the quantum-field nature of QCD (correlations, interference). They also provide new insights into spin structure of hadrons (spin-flip distributions, orbital angular momentum). GPDs are sensitive to chiral symmetry breaking effects, a fundamental property of QCD. Furthermore, GPDs unify existing ways of describing hadronic structure. The GPD formalism provides nontrivial relations between different exclusive reactions and also between exclusive and inclusive processes.

### 3.3 GPDs and transverse nucleon structure at collider energies

C. Weiss

Generalized parton distributions (GPDs) have emerged as a key concept in nucleon structure and the theory of high momentum-transfer processes in QCD. They unify the traditional notions of parton densities and elastic form factors and describe the transverse spatial distribution of quarks and gluons in a fast-moving hadron. A general introduction to GPDs and hard exclusive processes is given in section 3.2. Here we summarize the properties of GPDs at collider energies, where the parton picture can be combined with methods specific to high-energy scattering ("small-x physics"). This includes the transverse spatial structure of the nucleon at small $x$; gluon and quark imaging with hard exclusive processes at $e p$ colliders (HERA, EIC); the correspondence with the QCD dipole model and the role of transverse nucleon structure in saturation at small $x$; and the application of GPDs to high-energy $p p$ collisions with hard processes (Tevatron, LHC).

GPDs are defined as the transition matrix elements of the QCD twist- 2 operators between nucleon states of different momenta. They are functions of the longitudinal momentum fractions of the partons, $x$ and $x^{\prime}$, and the invariant momentum transfer $t$, as well as the resolution scale $Q^{2}$ (see figure 3.8a). Of particular interest is the "diagonal" limit $x=x^{\prime}$, where the momentum transfer is in the transverse direction only, $t=-|\boldsymbol{\Delta}|^{2}$, and the GPD can be regarded as the form factor of partons carrying longitudinal momentum fraction $x$. Its two-dimensional Fourier transform

$$
\begin{equation*}
f\left(x, b, Q^{2}\right) \equiv \int \frac{d^{2} \Delta}{(2 \pi)^{2}} e^{-i(\boldsymbol{\Delta} \boldsymbol{b})} \operatorname{GPD}\left(x, t=-\boldsymbol{\Delta}^{2}, Q^{2}\right) \tag{3.25}
\end{equation*}
$$

describes the transverse spatial distribution of partons with momentum fraction $x$ and thus provides a "tomographic" image of the structure of the fast-moving nucleon (see figure 3.8b) [580]. The coordinate $b$ measures the distance from the transverse center-of-mass (CM), defined as the average of the transverse positions of all constituents weighted with their longitudinal momentum fractions. In general, the removal of a parton with momentum fraction $x$ changes the position of the CM, and this effect must be taken into account in interpreting the coordinate distributions at $x \sim 1$. At $x \ll 1$ however, the contribution of the removed parton to the CM is negligible and one can think of the $b$-distributions of (3.25) as referring to a fixed transverse center of the nucleon. This considerably simplifies the spatial interpretation of GPDs at small $x$.


Figure 3.8. (a) GPD and partonic variables. (b) Transverse spatial distribution of partons. (c) QCD evolution generates small $x, x^{\prime}$ from the quasi-diagonal GPD at lower scale.


Figure 3.9. (left) Exclusive $J / \psi$ production as a probe of the gluon GPD. (right) Average transverse gluonic size of the nucleon $\left\langle b^{2}\right\rangle_{g}$ extracted from $J / \psi$ photoproduction at HERA [588, 589] and FNAL [590] (adapted from 591]). The effective scale at which the GPD is probed is $Q_{\text {eff }}^{2} \approx 3 \mathrm{GeV}^{2}$.

Hard exclusive processes require a nonzero longitudinal momentum transfer to the nucleon and probe the GPDs at $x-x^{\prime} \equiv$ $2 \xi \neq 0$, where the "skewness" is related to the Bjorken variable by $\xi=x_{B} /\left(2-x_{B}\right)$. Models or additional assumptions are generally needed to extract the diagonal GPD from the data. However, at $x_{B} \ll 1$ and sufficiently large $Q^{2}$ the "skewed" GPD can approximately be reconstructed from the diagonal limit 592, 593. In this case QCD evolution generates the GPD with $x$ and $x^{\prime}$ from configurations at a lower scale with momentum fractions $x_{0}, x_{0}^{\prime} \gg x, x^{\prime}$; because the difference of the parton momentum fractions is preserved under evolution, the lower-scale GPD is effectively evaluated in the diagonal limit $x_{0}-x_{0}^{\prime} \ll x_{0}, x_{0}^{\prime}$ (see figure 3.8k). This approximation allows one to relate the measured $t$-dependence of the differential cross sections directly to the transverse structure of the nucleon at fixed $x$.

The transverse spatial distribution of partons changes with the momentum fraction $x$ and the scale $Q^{2}$. The valence quarks and gluons at $x>0.1$ are concentrated at small transverse distances $b \ll 1 \mathrm{fm}$, as can be inferred from the nucleon axial form factor and exclusive processes at large $x$. Be-


Figure 3.10. A simulated measurement of exclusive $J / \psi$ electro-production with a mediumenergy EIC for an integrated luminosity of 100 $\mathrm{fb}^{-1}$. The expected statistical errors in the $t-$ dependence of the $J / \psi$ dilepton cross section in a fully differential measurement in $W, Q^{2}$ and $t$ are shown. The values of $x \equiv M_{J / \psi}^{2} / W^{2}$ in the bins are indicated above the curves, corresponding approximately to the $x$-values where the gluon GPD is probed. Such measurements can image the transverse distribution of gluons at $x>0.1$ and explore the unknown $t$-dependence at $|t|>1 \mathrm{GeV}^{2}$.
low $x<M_{\pi} / M_{N}$ chiral dynamics gives rise to a distinct large-distance contribution to the parton density at $b \sim 2 / M_{\pi}$ [594]. At even smaller values of $x$ the nucleon's transverse size is expected to grow as a result of Gribov diffusion in the successive parton branchings building up the small-x parton density. The transverse distribution also shrinks with increasing $Q^{2}$ as a result of DGLAP evolution [595. Overall, much interesting information on nucleon structure and non-perturbative dynamics can be obtained from the study of the transverse spatial distributions of quarks and gluons.

The transverse spatial distribution of gluons can be measured cleanly through exclusive $J / \psi$ photo- or electroproduction $\gamma^{(*)} N \rightarrow J / \psi+N$, or electroproduction of $\phi$ mesons at $Q^{2} \gtrsim 10 \mathrm{GeV}^{2}$ (see figure 3.9 a ). Measurements at HERA have confirmed the applicability of QCD factorization, with corrections for the finite size of the produced meson, and tested the universality of the gluon GPD; see 596 for a review. The data show that the nucleon's transverse gluonic radius at $x<0.01$ is substantially smaller than the transverse charge radius (see figure 3.9b). It increases only moderately with decreasing $x$, with a logarithmic slope much smaller than that of the Pomeron trajectory, $\alpha_{P}^{\prime}=0.25 \mathrm{GeV}^{-2}$, showing that Gribov diffusion is suppressed for partons with virtualities $\sim$ few $\mathrm{GeV}^{2}$. Both observations are of central importance for nucleon structure and small-x physics.

While the HERA experiments have provided basic information on the nucleon's transverse gluonic size at small $x$, many important questions remain unanswered:

- How are the gluons at $x>10^{-2}$ distributed in transverse space? Global PDF fits indicate a substantial momentum density of gluons in that $x$-range at low scales $Q^{2} \sim$ few $\mathrm{GeV}^{2}$. Knowledge of their spatial distribution would help to explain their dynamical origin, one of the key issues of nucleon structure in QCD.
- Do singlet quarks and gluons have the same transverse distribution? This can be studied by comparing the $t$-dependence of $J / \psi$ and $\phi$ with $\rho^{0}$ and $\gamma$ electroproduction. A larger radius for quarks than gluons is expected from non-perturbative effects 597.
- How are non-singlet sea quarks distributed in transverse space? The non-singlet sea at $x<0.1$ reveals non-perturbative QCD interactions (vacuum fluctuations, mesonic degrees of freedom) in the nucleon. This component is probed in exclusive $\pi, K, \rho^{+}$ or $K^{*}$ production - non-diffractive processes involving quantum number exchange.
- How does the nucleon's gluon GPD behave at $|t| \sim$ few $\mathrm{GeV}^{2}$ ? The large- $|t|$ behavior of GPDs is important not only to obtain accurate images at small $b$, but also to understand how soft Regge-like dynamics is connected to QCD at short distances.
- What is the probability for a nucleon to break up into a low-mass hadronic state ( $M_{H} \sim$ few GeV ) in an exclusive process at small $x_{B}$ ? Such "diffractive dissociation" reveals the quantum fluctuations of the nucleon's gluon density - new information going beyond the average densities described by the GPDs 598.

An EIC would enable a comprehensive program of transverse imaging of gluons and sea quarks in the nucleon. Measurements of $J / \psi$ photo- and electroproduction, as well as $\phi$ meson electroproduction at $Q^{2}>10 \mathrm{GeV}^{2}$, would cleanly map the transverse distribution of gluons, including the gluons at $x>0.1$ (see the example in figure 3.10). They could also explore the unknown $t$-dependence of the GPD at $|t|>1 \mathrm{GeV}^{2}$. Measurements of $\rho^{0}$ and $\gamma$ production (DVCS) would provide additional information on the singlet quarks. With a high-luminosity EIC, even the non-diffractive channels $\left(\pi, K, \rho^{+}, K^{*}\right)$ could be measured


Figure 3.11. (a) Dipole picture of high-energy scattering in the target rest frame. (b) Multiparton processes in high-energy $p p$ collisions.
for the first time down to $x \sim 0.01$, providing detailed information on the spatial distribution of the non-singlet sea, including its spin and flavor composition (see section 3.12).

The QCD factorization theorem for hard exclusive processes at small $x$ (figure 3.9a) is equivalent to the dipole picture of exclusive processes in the nucleon rest frame in the leading $\alpha_{s} \log Q^{2}$ approximation [599]. The scattering amplitude for a dipole of size $r$ with impact parameter $b$ is proportional to the $b$-dependent gluon density of (3.25) at a scale $Q^{2} \approx \pi^{2} / r^{2}$ (see figure 3.3a). This correspondence relates GPDs to the dipole model phenomenology of small- $x$ physics [596. In particular, the transverse spatial distribution of gluons is an essential input to studies of the unitarity limit in hard processes at small $x$ ("black-disk regime"). It defines the spatial profile of the initial conditions of non-linear QCD evolution equations leading to gluon saturation at small $x$. Detailed studies of saturation in the dipole model have used the transverse gluonic size extracted from the HERA data (see figure 3.9b) [600, 601; better knowledge of the transverse profile would help to accurately predict the $x$ and $b$-dependence of the saturation scale.

The transverse distribution of partons also plays an important role in high-energy $p p$ collisions with hard processes. It determines the probability of hard parton-parton processes as a function of the $p p$ impact parameter. Using knowledge of the transverse distribution of partons from $e p$ scattering one can explain many features of the underlying event in $p p$ collisions with hard processes [591]. In particular, one can predict the rate of multiparton processes (see figure 3.3b), which form a potentially large background to new physics events at the LHC. The enhancement of such processes beyond their geometric probability signals dynamical correlations between partons, the study of which represents a new frontier of nucleon structure.

### 3.4 How large can the distributions $E^{q}$ and $E^{g}$ be?

Markus Diehl

### 3.4.1 Positivity bounds

The generalized parton distributions $E$ for quarks and gluons play a key role in the study of nucleon structure through exclusive processes. In the following I focus on the case of zero skewness, $\xi=0$, where the physics interpretation is most intuitive and where constraints on these distributions are most easily obtained. The density of unpolarized quarks in a proton polarized along the $x$-axis is given by

$$
\begin{equation*}
q^{X}(x, \vec{b})=q\left(x, b^{2}\right)-\frac{b^{y}}{m} \frac{\partial}{\partial b^{2}} e_{q}\left(x, b^{2}\right), \tag{3.26}
\end{equation*}
$$

where $m$ is the proton mass. The quarks have impact parameter $\vec{b}$ and move in the $z$ direction with momentum fraction $x$. The term with

$$
\begin{equation*}
e_{q}\left(x, b^{2}\right)=\int \frac{d^{2} \Delta}{(2 \pi)^{2}} e^{-i \vec{b} \vec{\Delta}} E^{q}\left(x, \xi=0, t=-\vec{\Delta}^{2}\right) \tag{3.27}
\end{equation*}
$$

quantifies the transverse shift of the density due to the proton polarization. The density interpretation of (3.26) (together with its analog for longitudinal quark and proton polarization) entails a positivity bound [602]:

$$
\begin{equation*}
\frac{b^{2}}{m^{2}}\left[\frac{\partial}{\partial b^{2}} e_{q}\left(x, b^{2}\right)\right]^{2} \leq\left[q\left(x, b^{2}\right)+\Delta q\left(x, b^{2}\right)\right]\left[q\left(x, b^{2}\right)-\Delta q\left(x, b^{2}\right)\right] \tag{3.28}
\end{equation*}
$$

The theoretical status of this bound is the same as for the positivity of unpolarized parton densities and for the Soffer inequality: they hold in the parton model and are preserved by leading-order DGLAP evolution to higher scales, but they can be violated by higher-order evolution effects or at very low scales. Since so little is known about $E$, I suggest to use (3.28) as a guide, with proper caution. A consequence of (3.28) is that $\left(\partial / \partial b^{2}\right) e_{q}$ must decrease faster with $b$ than $\sqrt{q^{2}-\Delta q^{2}}$. This has immediate consequences for parameterizations: using Gaussian forms $E^{q} \propto e^{B_{e} t}$ and $\sqrt{q^{2}-\Delta q^{2}} \propto e^{B_{q} t}$ for the momentum-space distributions at $\xi=0$, one must have $B_{e}<B_{q}$, and with power laws $E^{q} \propto\left(1-t / M_{e}^{2}\right)^{-3}$ and $\sqrt{q^{2}-\Delta q^{2}} \propto\left(1-t / M_{q}^{2}\right)^{-2}$, one must have $1 / M_{e}<1 / M_{q}$, with equality of the parameters not being allowed in either case. Starting from (3.28) one can also derive a bound 602 for the integrated distribution:

$$
\begin{equation*}
e_{q}(x)=\int d^{2} b e_{q}\left(x, b^{2}\right)=E^{q}(x, \xi=0, t=0) . \tag{3.29}
\end{equation*}
$$

That bound constrains the large $x$ behavior of $e_{q}(x)$, but numerically turns out to be rather weak for $x$ below 0.5 , see e.g. 603].

Analogous definitions and bounds apply to antiquark and gluon distributions $e_{\bar{q}}$ and $e_{g}$.

### 3.4.2 Sum rules

An important constraint follows from the sum rule

$$
\begin{equation*}
\kappa_{q}=\int_{0}^{1} d x\left[e_{q}(x)-e_{\bar{q}}(x)\right] \tag{3.30}
\end{equation*}
$$



Figure 3.12. GPDs in the forward limit obtained in a phenomenological fit 582 to the nucleon form factors. The first two panels correspond to two parameter sets giving a good fit. The valence quark distributions $u_{\mathrm{val}}=u-\bar{u}$ and $d_{\mathrm{val}}=d-\bar{d}$ in the third panel are shown for comparison. All distributions are shown at the scale $\mu=2 \mathrm{GeV}$.
where $\kappa_{q}$ is the contribution of quark flavor $q$ to the anomalous magnetic moment of the proton. From the magnetic moments of proton and neutron one obtains $\kappa_{u}-\kappa_{d}=3.71$ and $\kappa_{u}+\kappa_{d}+\kappa_{s}=-0.36$. Under the reasonable assumption that $\kappa_{s}$ is small compared with $\kappa_{u}$ and $\kappa_{d}$, these numbers imply that $\kappa_{u}$ and $\kappa_{d}$ are both large but have opposite signs and largely cancel in the flavor sum. As a consequence, the functions $e_{u, \text { val }}(x)=e_{u}(x)-e_{\bar{u}}(x)$ and $e_{d, \text { val }}(x)=e_{d}(x)-e_{\bar{d}}(x)$ must be large at least in some region of $x$. This is illustrated in figure 3.12, which shows distributions obtained by fitting a model ansatz for $u$ and $d$ quark GPDs to the electromagnetic nucleon form factors [582] (neglecting strange-quark contributions). The fit suggests that $e_{u, \mathrm{val}}$ and $e_{d, \mathrm{val}}$ are of similar size as the unpolarized valence distributions, whereas $e_{u, \mathrm{val}}+e_{d, \text { val }}$ is small and poorly known, to the point that we do not know whether it has zero crossings.

The second moments of $e(x)$ appear in Ji's angular momentum sum rules,

$$
\begin{equation*}
2 J^{q}=\int_{0}^{1} d x x[q(x)+\bar{q}(x)]+\int_{0}^{1} d x x\left[e_{q}(x)+e_{\bar{q}}(x)\right], \quad 2 J^{g}=\int_{0}^{1} d x x g(x)+\int_{0}^{1} d x x e_{g}(x) \tag{3.31}
\end{equation*}
$$

where they give "nontrivial" contributions in addition to the "trivial" ones from the momentum integrals of quarks and gluons (whose values are well known). Summed over all partons, the momentum integrals add up to 1 and the angular momenta to $\frac{1}{2}$, so that

$$
\begin{equation*}
\int_{0}^{1} d x x e_{\operatorname{sing}}(x)+\int_{0}^{1} d x x e_{g}(x)=0 \tag{3.32}
\end{equation*}
$$

where $e_{\text {sing }}(x)=\sum_{q}\left[e_{q}(x)+e_{\bar{q}}(x)\right]$. Note that both (3.30) and (3.32) are exact relations in QCD, in contrast to the positivity bound (3.28). The scale dependence of $e_{g}(x)$ and $e_{\text {sing }}(x)$ is governed by coupled DGLAP equations, with the same kernels as for the unpolarized gluon and quark singlet distributions. With (3.32) one finds that to leading order in $\alpha_{s}$

$$
\begin{equation*}
\int_{0}^{1} d x x e_{g}(x, \mu)=\left(\frac{\alpha_{s}(\mu)}{\alpha_{s}\left(\mu_{0}\right)}\right)^{\gamma} \int_{0}^{1} d x x e_{g}\left(x, \mu_{0}\right) \tag{3.33}
\end{equation*}
$$

where $\gamma=50 / 81$ for $n_{f}=3$ and $56 / 75$ for $n_{f}=4$ active flavors. All numbers in the following refer to $\mu=2 \mathrm{GeV}$; the evolution of (3.33) to higher scales is rather slow.

With the distributions in 582 one finds that $\int d x x e_{\text {sing }}$ has a very small valence part $\int d x x\left[e_{u}-e_{\bar{u}}+e_{d}-e_{\bar{d}}\right]$ between -0.042 and 0.068. A similar situation is found in lattice calculations, which obtain a small contribution to $\int d x x\left[e_{u}+e_{\bar{u}}+e_{d}+e_{\bar{d}}\right]$ from connected graphs, with values between $-0.077(16)$ and $0.015(11)$ for different extrapolations to the physical quark masses 604].

Assuming that $\int d x x\left[e_{u}-e_{\bar{u}}+e_{d}-e_{\bar{d}}\right]$ is indeed small (and barring the possibility of an implausibly large $e_{s}-e_{\bar{s}}$ ) we find that the sum $\int d x x e_{g}+\int d x x e_{\text {sea }}$ of second moments must be small, where $e_{\text {sea }}=2 \sum_{q} e_{\bar{q}}$. This still leaves us with a number of possible scenarios:

1. both $e_{g}(x)$ and $e_{\text {sea }}(x)$ are small (note that this does not exclude large $e_{\bar{q}}(x)$ for individual quark flavors: only the flavor sum must be small),
2. $e_{g}(x)$ and $e_{\text {sea }}(x)$ are both large but have opposite signs,
3. both distributions are large but have nodes such that their second moments are small.

Scenario 2 is illustrated in figure 3.13, which shows two variants of model distributions proposed in 605. The absolute size of the distributions is limited by the bound (3.28) and its analogs for $e_{\bar{q}}$ and $e_{g}$, and the opposite signs of $e_{g}$ and $e_{\text {sea }}$ ensure that (3.32) can be fulfilled. We see that scenarios where both $e_{g}$ and $e_{\text {sea }}$ are large cannot be ruled out with our present knowledge. If the above model distributions are evolved to higher scales, $e_{g}$ becomes even larger and steeper at small $x$ 603].


Figure 3.13. Two variants of model distributions $e_{g}$ and $e_{\text {sing }}$ at $\mu=2 \mathrm{GeV}$ from 605]. The distributions of the quark singlet $q_{\text {sing }}=\sum_{q}(q+\bar{q})$ and the gluon are shown for comparison.

### 3.4.3 Exclusive processes

Up to now I discussed $E^{q}, E^{\bar{q}}$ and $E^{g}$ at zero skewness $\xi=0$, but in exclusive processes like DVCS and meson production $\xi$ is always nonzero. Nevertheless, experience from phenomenology and models suggests that GPDs at $\xi=0$ are closely enough related to those at $\xi \neq 0$ to serve as a guide for their overall size, see e.g. [577, 606].

Note that even the large model distributions $e_{g}$ and $e_{\text {sea }}$ in figure 3.13 result in small values for the transverse target spin asymmetry $A_{U T}$ in exclusive $\rho$ electroproduction [605]. This is in part due to cancellations in the sum over $u$ and $d$ quarks in this process (the
same distributions give a larger asymmetry for $\omega$ production). Moreover, $A_{U T}$ in exclusive meson production is proportional to $\operatorname{Im}\left(\mathcal{H} \mathcal{E}^{*}\right)$, where $\mathcal{H}$ and $\mathcal{E}$ are the scattering amplitudes associated with $H$ and $E$ distributions, respectively. Hence $A_{U T}$ is also small when both amplitudes are large but have a small relative phase. The transverse target asymmetry in DVCS is therefore of special importance, because the interference between Compton scattering and the Bethe-Heitler process is linear in $\operatorname{Im} \mathcal{E}$.

### 3.5 Imaging transverse distributions

Gerald A. Miller

### 3.5.1 Introduction

Much effort has gone into measuring electromagnetic form factors, which are related to the charge and magnetization densities within the nucleons. The influence of relativistic motion of the quarks within the nucleon causes the standard textbook interpretation of form factors as three-dimensional Fourier transforms to be wrong 607. The use of transverse densities [608, 609] avoids various difficulties by working in the infinite momentum frame and taking the spacelike momentum transfer to be in the direction transverse to that of the infinite momentum. In this case, the different momenta of the initial and final nucleon states are accommodated by using two-dimensional Fourier transforms and transverse charge and magnetization densities are constructed from density operators that are the absolute square of quark-field operators.

The transverse charge density is given by [608, 610]

$$
\begin{equation*}
\rho(b)=\int d x^{-} \rho\left(x^{-}, b\right)=\frac{1}{2 \pi} \int Q d Q J_{0}(Q b) F_{1}\left(Q^{2}\right), \tag{3.34}
\end{equation*}
$$

where $\rho\left(x^{-}, b\right)$ is the three dimensional spatial density.
The transverse charge densities are shown in [608, 609]. The interesting feature is that the central neutron charge density is negative. An interpretation of this finding based on the impact parameter distribution [580, 611 was presented in 612]. All models of these quantities are based on the Drell-Yan-West relation, which connects large values of $x$ with large values of $Q^{2}$. These models tell us that the $d$ quarks that dominate deep inelastic scattering from the neutron at large values of $x$ dominate the neutron center. It is also possible that the negatively charge pionic cloud may penetrate the center [613].

The transverse anomalous magnetization density is obtained from the matrix element of the magnetization density operator $\frac{1}{2} \vec{b} \times \vec{j}$, where $\vec{j}$ is taken in the $z$-direction:

$$
\begin{equation*}
\rho_{M}(b)=\frac{\sin ^{2} \phi}{2 M} b \int \frac{Q^{2} d Q}{2 \pi} F_{2}\left(Q^{2}\right) J_{1}(Q b) . \tag{3.35}
\end{equation*}
$$

The integral $\int d^{2} b \rho_{M}(b)$ gives the anomalous magnetic moment.

### 3.5.2 Realistic transverse images of the proton charge and magnetic densities

The word "realistic" refers to the ability to know the uncertainty in the transverse densities derived from experiment. The previously obtained transverse densities are derived from various parameterizations of the form factors. A more detailed treatment is needed to be able to extract uncertainties. The following discussion is based on the analysis 614.

The basic idea behind our approach is to use the observation that $\rho(b) \approx 0$ for $b \geq R$, where $R$ is a finite distance. Since the functions $\rho$ and $F$ are Fourier transforms, $F$ is bandlimited. We proceed in the spirit of the Nyquist-Shannon sampling theorem and expand the function $\rho$ as

$$
\begin{equation*}
\rho(b)=\sum_{n=1}^{\infty} \frac{1}{2 \pi} \frac{2}{R^{2} J_{1}\left(X_{n}\right)^{2}} F\left(Q_{n}^{2}\right) J_{0}\left(X_{n} \frac{b}{R}\right), \tag{3.36}
\end{equation*}
$$



Figure 3.14. Plot of $\rho_{D}$ (solid), 5 term approximation (red, long dash), 10 term approximation (green, medium dash) and 15 term approximation (brown, short dash). From Ref. 614].
where $X_{n}$ is the $n$-th zero of the regular cylindrical Bessel function of order $0, J_{0} ; Q_{n} \equiv$ $X_{n} / R$ and $X_{n} \approx(n+3 / 4) \pi$. Equation (3.36) defines the so-called finite radius approximation (FRA). Using, for example, $R=3 \mathrm{fm}$ and $n=10, Q_{n}^{2} \approx 4 \mathrm{GeV}^{2}$. Thus, the measurement up to $Q^{2}=4 \mathrm{GeV}^{2}$ determines the first ten terms of the expansion. As an example, let us consider the expansion (3.36) for the dipole form factor: $F_{D}\left(Q^{2}\right)=1 /\left(1+Q^{2} / \Lambda^{2}\right)^{2}$ with $\Lambda^{2}=0.71 \mathrm{GeV}^{2}$. The results shown in figure 3.14 indicate that relatively few terms suffice to give an accurate representation.

The relationship between the FRA and the usual expansion into a complete set of functions is examined in 614 where it is shown that the FRA is very accurate. The available data set consists of ep scattering up to $31 \mathrm{GeV}^{2}$ and $G_{E, M}$ are separately extracted for up to $10 \mathrm{GeV}^{2}$. The form factors $G_{E}$ and $G_{M}$ have been extracted from a global analysis of the world's cross section and polarization data, including corrections for two-photon exchange corrections [615]. The analysis is largely identical to that of 616], although additional high $Q^{2}$ form factor results [617] have been included. In addition, the slopes of $G_{E}$ and $G_{M}$ at $Q^{2}=0$ were constrained in the global fit based on a dedicated analysis of the low $Q^{2}$ data. In writing $G_{E}\left(Q^{2}\right)=1-Q^{2} R_{E}^{2} / 6$, the value of $R_{E}$ was constrained to be 0.878 fm and $R_{M}$ was constrained to be 0.860 fm . This is important in the extraction of the large scale structure of the density. The fit is given in 614.

We then use the fit and uncertainties for $G_{E}$ and $G_{M}$ to extract $F_{1}$ and $F_{2}$, treating the uncertainties in $G_{E}$ and $G_{M}$ as uncorrelated, yielding:

$$
\begin{align*}
& \left(d F_{1}\right)^{2}=\left(\frac{1}{1+\tau}\right)^{2}\left(d G_{E}\right)^{2}+\left(\frac{\tau}{1+\tau}\right)^{2}\left(d G_{M}\right)^{2}, \\
& \left(d F_{2}\right)^{2}=\left(\frac{1}{1+\tau}\right)^{2}\left(d G_{E}\right)^{2}+\left(\frac{1}{1+\tau}\right)^{2}\left(d G_{M}\right)^{2} . \tag{3.37}
\end{align*}
$$

For $Q^{2}<30 \mathrm{GeV}^{2}$, we use $d F_{1}$ above in the FRA to get $d \rho(b)$. For $Q^{2}>30 \mathrm{GeV}^{2}$, we use the FRA and take $d F_{1}= \pm \mid F_{1}$ (fit)|. This corresponds to a maximum value of $n=30$. The resulting transverse charge density is shown in figure 3.15. The proton transverse charge density is now very well known.

Our FRA technique can be exploited to image other quantities that depend on the transverse position. Suppose there is a transverse quantity $\rho^{(\lambda)}(b)$ that is a two-dimensional


Figure 3.15. (Color online) $\rho_{c h}$ (solid, blue) with error bands (short dashed, red). From Ref. 614].

Fourier transform of an experimental observable $F^{(\lambda)}\left(Q^{2}\right)$ such that

$$
\begin{equation*}
\rho^{(\lambda)}(b)=\frac{1}{2 \pi} \int Q d Q J_{\lambda}(Q b) F^{(\lambda)}\left(Q^{2}\right) . \tag{3.38}
\end{equation*}
$$

An example, discussed in detail in [614], is the magnetization density $\rho_{M}$. The index $(\lambda)$ is associated with a given number of units of the orbital angular momentum. The extraction of $\rho^{(\lambda)}(b)$ is facilitated by using the expansion

$$
\begin{equation*}
\rho^{(\lambda)}(b)=\sum_{n=1}^{\infty} \frac{2}{R^{2} J_{\lambda+1}\left(X_{\lambda, n}\right)^{2}} F^{(\lambda)}\left(Q_{\lambda, n}^{2}\right), J_{\lambda}\left(X_{\lambda, n} \frac{b}{R}\right), \tag{3.39}
\end{equation*}
$$

where $X_{\lambda, n}$ is the $n$-th zero of the Bessel function of order $\lambda ; Q_{\lambda, n}=X_{\lambda, n} / R$. The result (3.39) can be used to relate accessible kinematic ranges with transverse regions.

### 3.5.3 Summary

Much data for form factors exist and JLab12 will further improve the data set. The charge density is not a three-dimensional Fourier transform of $G_{E}$. One can interpret form factors as determining transverse charge and magnetization densities. The nucleon transverse densities are known now to high precision. The new FRA technique can be used for other quantities that depend on transverse position, in particular, for the exclusive scattering amplitudes and generalized parton distributions discussed in this chapter.
Acknowledgments. I thank S. Venkat, J. Arrington, and X. Zhan for their extensive efforts in producing the paper [614] on which this presentation is based. I also wish to thank Jefferson Laboratory for its hospitality during a visit while this work was being completed.

### 3.6 From transverse-momentum spectra to transverse images

Elke-Caroline Aschenauer, Markus Diehl, Salvatore Fazio

### 3.6.1 Imaging partons in the transverse plane

The principle of "parton imaging" using exclusive processes such as DVCS or hard exclusive meson production is rather simple. The key variable to measure is the transverse momentum transfer $\vec{\Delta}_{T}$ to the target proton or nucleus in the $\gamma^{*}$-target c.m. The invariant momentum transfer is then given by

$$
\begin{equation*}
t=-\frac{x^{2} m^{2}+\vec{\Delta}_{T}^{2}}{1-x} \quad \text { with } \quad x=\frac{Q^{2}+M_{V}^{2}}{Q^{2}+W^{2}} \tag{3.40}
\end{equation*}
$$

where $m$ is the target mass and $M_{V}$ the mass of the produced meson. For DVCS one should omit $M_{V}$, so that $x$ coincides with the Bjorken variable. In the limit of large $Q^{2}+M_{V}^{2}$, the $\gamma^{*} p$ scattering amplitude is a linear combination of generalized parton distributions convoluted with hard-scattering kernels. The distribution of partons in the transverse plane is obtained by a Fourier transform w.r.t. $\vec{\Delta}_{T}$ [580, 611]. In the simple case where the unpolarized quark or gluon GPDs $H^{i}$ dominate the $\gamma^{*} p$ cross section $d \sigma / d t$, the impact parameter profile is

$$
\begin{equation*}
F\left(b, x, Q^{2}\right) \propto \frac{1}{(2 \pi)^{2}} \int d^{2} \vec{\Delta}_{T} e^{-i \vec{b} \vec{\Delta}_{T}} \sqrt{\frac{d \sigma}{d t}}=\frac{1}{2 \pi} \int_{0}^{\infty} d \Delta_{T} \Delta_{T} J_{0}\left(b \Delta_{T}\right) \sqrt{\frac{d \sigma}{d t}}, \tag{3.41}
\end{equation*}
$$

where $\Delta_{T}=\left|\vec{\Delta}_{T}\right|$ and $b=|\vec{b}|$. For simplicity we drop the information from the absolute size of the cross section in this contribution and focus our attention on the normalized $b$-space profile, which satisfies $\int d^{2} b F\left(b, x, Q^{2}\right)=1$. For polarization asymmetries and for the interference term between DVCS and the Bethe-Heitler process, the extraction of the relevant $\gamma^{*} p$ amplitudes is more involved, but the principle of Fourier transforming these amplitudes w.r.t. $\vec{\Delta}_{T}$ remains the same.

In the present contribution, we estimate how accurately one can hope to determine $F\left(b, x, Q^{2}\right)$ from cross section measurements for DVCS on the proton. Firstly, $d \sigma / d t$ will have statistical and systematic errors. Secondly, the range of $\Delta_{T}$ in a measurement will be restricted both from above and from below, so that an extrapolation is required in order to perform the Fourier integral in (3.41).

### 3.6.2 Acceptance in transverse momentum

To achieve the precision discussed below for imaging partons in the impact parameter space, it is critical to integrate from the beginning the detection of the scattered proton into the detector and interaction region design. The scattered proton in exclusive reactions is characterized by carrying almost the full beam momentum and a transverse momentum $\Delta_{T}$ between several MeV and a few GeV , corresponding to very small scattering angles. Figure 3.16 shows the relation between the longitudinal momentum of the protons and their scattering angle for two different ep center-of-mass energies.

The commonly used method to detect these protons is to integrate "Roman pots" in the machine lattice. The standard technologies for such detectors are silicon strip detectors or


Figure 3.16. (Color online) The longitudinal momentum $p_{z}$ of the scattered proton in exclusive reactions vs. its scattering angle $\theta$ for an $e p$ center-of-mass energy of 15.5 GeV (left) and 145 GeV (right).
scintillating fiber detectors. The acceptance for protons with the transverse momentum in the MeV region is limited by the requirement that Roman pots must have a beam clearance distance of 10 times the beam emittance. The upper transverse acceptance is given by the apertures of the magnets that the protons have to transverse. For transverse momenta above 1 GeV , the proton can be detected in the main solenoidal detector. Details on the solutions for the eRHIC and ELIC interaction region designs are given in section 7.3,

### 3.6.3 Precision of the measurement

A detailed simulation of DVCS events is described in section 3.9. To illustrate the expected statistical accuracy of a measurement, we show $d \sigma / d t$ for a selected bin of $x$ and $Q^{2}$ in figure 3.17. The value of $y$ in this bin ranges from 0.05 to 0.14 . For bins with lower $x$ or lower $Q^{2}$, the statistical errors are smaller, except for kinematics where the $y>0.01$ cut applied in the simulation becomes relevant.

The $t$ spectrum shown in the figure 3.17 was generated with an exponential dependence $d \sigma / d t \propto \exp (B t)$ with $B=5 \mathrm{GeV}^{-2}$. An exponential fit to the generated spectrum gives $B=5.02 \mathrm{GeV}^{-2}$ with an error below $1 \%$. Data of this quality also allows one to explore possible deviations from an exponential spectrum. To this end, we have also fitted to $d \sigma / d t \propto \exp \left(B t-C t^{2}\right)$. This fit and its $1 \sigma$ error band is shown in the figure and gives $B=(4.92 \pm 0.10) \mathrm{GeV}^{-2}$ and $C=(0.079 \pm 0.076) \mathrm{GeV}^{-4}$. Although the relative uncertainty on the extra parameter $C$ is large, the term $C t^{2}$ in the exponential is small compared with $B t$ in the fitted $t$ range (as it should be for a spectrum generated with a pure exponential law). The logarithmic $t$ slope at $|t|=1.75 \mathrm{GeV}^{2}$ in this fit is $(5.20 \pm 0.18) \mathrm{GeV}^{-2}$.

We conclude at this point that with the projected luminosity available at an EIC, the $t$ spectrum for the DVCS cross section will be dominated by systematic uncertainties and not


Figure 3.17. (Color online) Generated $t$ spectrum for the DVCS cross section in a selected bin of $x$ and $Q^{2}$. The errors are statistical only and correspond to the integrated luminosity of $11.9 \mathrm{fb}^{-1}$ for $|t|<1 \mathrm{GeV}^{2}$ and to $151 \mathrm{fb}^{-1}$ for $|t|>1 \mathrm{GeV}^{2}$. The curve represents a fit explained in the text.
by statistics, even if one measures differentially in $x$ and $Q^{2}$. Systematic uncertainties, for instance due to momentum resolution, strongly depend on details of the experimental setup and have not been studied yet. We note that the normalized $b$ space profile $F\left(b, x, Q^{2}\right)$ is not affected by errors on the overall luminosity and acceptance.

### 3.6.4 Uncertainty from the extrapolation in $t$

We now estimate the uncertainty in the impact parameter profile $F(b)$ due to the lack of knowledge of the scattering amplitude for all $t$. Since the projected statistical errors are so small, we do not include them in this exercise.

For the extrapolation to large $|t|$, we assume a measured $t$-spectrum $d \sigma / d t \propto \exp (B t)$ with $B=4 \mathrm{GeV}^{-2}$ up to $|t|_{\max }=1$ or $2 \mathrm{GeV}^{2}$. Larger values of $B$ give a smaller cross section at high $|t|$ and thus a smaller extrapolation uncertainty in the Fourier integral (3.41). In turn, the statistical errors on the cross section at high $|t|$ are then larger, so that in $F(b)$ there is a tradeoff between the uncertainties from the measured $t$ spectrum and those from its extrapolation.

To estimate the extrapolation uncertainty, we adopt a strategy similar to that in 618] and assume different forms for the scattering amplitude (i.e., for $\sqrt{d \sigma / d t}$ ) at $|t|>|t|_{\max }$ :

1. an exponential $\propto \exp (B t / 2)$, labeled "exp" in figure 3.18
2. a dipole form $\propto\left(1+|t| / M^{2}\right)^{-2}$, labeled "dip",
3. a modified dipole form $\propto\left(1+0.05|t| / M^{2}\right)^{-1}\left(1+0.45|t| / M^{2}\right)^{-1}$, labeled "mod dip",
4. a modified exponential $\propto \exp \left(-D t^{2}\right)$, labeled "mod exp".

In each case we require the amplitude and its first derivative to be continuous at $|t|=|t|_{\max }$. Note that in the measured $t$ region, forms 2 to 4 would give unacceptable fits to the simulated spectrum in figure 3.17. Forms 3 and 4 should be regarded as examples for functions falling off especially slowly or especially fast and do not claim to be particularly realistic. When performing the Fourier transform (3.41), we neglect the term $x^{2} m^{2}$ in (3.40), which is justified in a large region of phase space.

In figure 3.18 we show the resulting scattering amplitude (normalized to unity at $\vec{\Delta}_{T}=$ $\overrightarrow{0}$ ) and its Fourier transform $F(b)$. We observe that the curves in $b$ space are close together in a wide region and rather quickly start to differ below a certain critical value $b_{\text {cr }}$. For $|t|_{\max }=$ $1 \mathrm{GeV}^{2}$, we find $b_{\text {cr }} \sim 0.25 \mathrm{fm}$ and an appreciable spread of $F(b)$ at lower $b$. This would be a serious limitation for studying the central region of the proton. Interesting physical effects like the variation of $F(b)$ with $x$ or $Q^{2}$ are typically expected to be only logarithmic (see, e.g., the estimates in [619]) and hence require sufficiently precise measurements. Clearly, there is a very significant gain of accuracy in impact parameter space if $|t|_{\max }$ can be raised from 1 to $2 \mathrm{GeV}^{2}$, i.e., if a scattered proton in the corresponding kinematics can be seen in the main detector. We then find $b_{\text {cr }} \sim 0.1 \mathrm{fm}$ and a small uncertainty even at $b=0$.

As an alternative scenario we assume a dipole form instead of an exponential $t$ dependence in the measured region 1 with a dipole mass $M=770 \mathrm{MeV}$ that gives the same scattering amplitude at $|t|=1 \mathrm{GeV}^{2}$ as the exponential with $B=4 \mathrm{GeV}^{-2}$. The extrapolation error is larger in the dipole scenario, but since the cross section decreases much more slowly, it can be measured out to higher values of $|t|$ before statistics becomes an issue. We recall however that a description in terms of generalized parton distributions requires $|t| \ll Q^{2}+M_{V}^{2}$. As seen in figure 3.19, a measurement up to $|t|_{\max }=3.3 \mathrm{GeV}^{2}$ in the dipole scenario gives a very precise $F(b)$ down to $b_{\text {cr }} \sim 0.1 \mathrm{fm}$. The extrapolation uncertainty at lower $b$ is larger than for $|t|_{\max }=2 \mathrm{GeV}^{2}$ in the exponential scenario.

Let us now investigate the extrapolation to small $|t|$. We assume again an exponential cross section $d \sigma / d t \propto \exp (B t)$, but now with a larger slope $B=6.6 \mathrm{GeV}^{-2}$ in order to maximize the importance of low $|t|$ in the Fourier integral. We consider either 300 MeV or 200 MeV as minimum measured values of $\Delta_{T}$, and take the following extrapolations for $\Delta_{T}$ down to zero:

1. an exponential in $t$, labeled "exp" in figure 3.20.
2. a dipole form $\propto\left(1+|t| / M^{2}\right)^{-2}$, labeled "dip",
3. a linear function in $t$, labeled "lin",
4. a monopole form $\propto\left(1+|t| / M^{2}\right)^{-1}$, labeled "mono",
5. an inverse square root $\propto\left(1+|t| / M^{2}\right)^{-1 / 2}$, labeled "sqrt".

We see in figure 3.20 that with a measurement down to $\Delta_{T}=300 \mathrm{MeV}$, one has a rapidly growing extrapolation uncertainty for $b$ above about 1.25 fm . The situation dramatically improves if one has to extrapolate only below $\Delta_{T}=200 \mathrm{MeV}$. Repeating this study with a dipole form in the measured region yields the same conclusion 621]. Whether a measurement down to even lower $\Delta_{T}$ can still improve the accuracy of $b$ space images can only be decided after an estimate of experimental uncertainties.

Let us recall the specific physics interest of the impact parameter profile of the proton at very large $b$. This is the region where the dynamics of chiral symmetry breaking should manifest itself. A description in terms of virtual pion fluctuations yields definite predictions, such as a behavior $F(b) \propto b^{-1} e^{-\kappa b}$ with $\kappa \approx 2 m_{\pi} \approx(0.7 \mathrm{fm})^{-1}$ at large $b$ 594. This translates into a small $|t|$ behavior given by the inverse square root law in point 5 (with $M^{2}=\kappa^{2}$ ). These predictions should be tested quantitatively.

[^271]

Figure 3.18. (Color online) Examples for normalized amplitudes (left) with different extrapolations to large $|t|$, together with their Fourier transforms to impact parameter space (right).


Figure 3.19. (Color online) As in figure 3.18 but with a dipole form of the amplitude up to $|t|=$ $3.3 \mathrm{GeV}^{2}$.


Figure 3.20. (Color online) As in figure 3.18, but with extrapolation to small $|t|$, i.e. small $\Delta_{T}$. The impact parameter profile $F(b)$ is multiplied with $b^{2}$ in order to make the large $b$ behavior visible.

In summary, we find that with the parameters we have assumed, neither statistics nor acceptance in $t$ will seriously limit $b$ space imaging at an EIC, with an accessible $b$ range from 0.1 fm up to 1.5 fm or larger. Detailed estimates of experimental uncertainties will be necessary to assess the limiting factors of accuracy in this endeavor.

### 3.7 GPDs from DVCS

Matthias Burkardt, Hikmat BC

### 3.7.1 Introduction

GPDs are linked to many processes and observables involving hadrons [622], but their most intuitive application is in the context of Ji's angular momentum decomposition (see section (3.4) and in three-dimensional imaging (see section (3.6). Both involve GPDs in the $\xi=0$ limit (the $\xi$-dependence drops out in the Ji sum rule). At the same time, the DVCS amplitude $\mathcal{A}_{\text {DVCS }}$ provides direct access only to GPDs along the "diagonal" $x=\xi$ (through the imaginary part of the DVCS amplitude) as well as to a convolution integral involving GPDs (through the real part of $\mathcal{A}_{\mathrm{DVCS}}$ ). In the leading order (LO) factorization, one finds

$$
\begin{align*}
\Im m \mathcal{A}_{\mathrm{DVCS}} & \longrightarrow G P D^{(+)}(\xi, \xi, t), \\
\Re e \mathcal{A}_{\mathrm{DVCS}} & \longrightarrow \int_{-1}^{1} d x \frac{G P D^{(+)}(x, \xi, t)}{x-\xi} . \tag{3.42}
\end{align*}
$$

The ' $(+)^{\prime}$ ' superscript in (3.42) emphasizes that DVCS is sensitive only charge-even (i.e., quark+antiquark) combinations of GPDs. Moreover, the accessible range in $\xi$ is limited, $\xi_{\min }<\xi<\xi_{\max }$. The lower limit $\xi_{\min }$ is defined by the DIS kinematics. The upper limit $\xi_{\text {max }}$ follows from the relation

$$
\begin{equation*}
-t=\frac{4 \xi^{2} M^{2}+\Delta_{\perp}^{2}}{1-\xi^{2}}, \tag{3.43}
\end{equation*}
$$

and the positivity of $\boldsymbol{\Delta}_{\perp}^{2}$. Thus, even in an idealized DVCS experiment (fixed $Q^{2}$ ), where angular dependencies as well as spin asymmetries have been used to disentangle different GPDs and the proton and 'neutron' targets have been used to accomplish the flavor decomposition, one can at best expect a determination of the observables in (3.42) for $\xi_{\text {min }}<\xi<\xi_{\text {max }}$. One of the key question in the context of DVCS is whether this information will allow an unambiguous and model-independent extraction of GPDs.

### 3.7.2 Constraints on GPDs: polynomiality, dispersion relations and QCD evolution

GPDs are not only constrained by DVCS, but also by DIS and form factor data. However, the form factor data constrains only charge-odd distributions and helps only in kinematical regimes where antiquark contributions are negligible. While DIS data is sensitive to charge-even distributions, there is no DIS data that would constrain the forward ( $\xi=0$, $t=0)$ limit of $E^{q}(x, \xi, t)$.

Fortunately, multiple theoretical constraints exist that will be helpful in determining GPDs from DVCS data. For example, Lorentz invariance implies the polynomiality conditions on GPDs [274, 574]:

$$
\begin{equation*}
\int_{-1}^{1} d x x^{n} G P D(x, \xi, t)=A_{n, 0}(t)+A_{n, 2}(t) \xi^{2}+\ldots+A_{n, n+1} \xi^{n+1} \tag{3.44}
\end{equation*}
$$

where the highest power $\xi^{n+1}$ is only present when $n$ is odd. These polynomiality conditions imply that the dependence of GPDs on the variables $x$ and $\xi$ cannot be independent. This imposes significant and rigorous constraints on any GPD extraction from DVCS data.

Rigorous dispersion relations exist for the DVCS amplitude $\mathcal{A}\left(\nu, t, Q^{2}\right)$ :

$$
\begin{equation*}
\Re e \mathcal{A}\left(\nu, t, Q^{2}\right)=\frac{\nu^{2}}{\pi} \int_{0}^{\infty} \frac{d \nu^{\prime 2}}{\nu^{\prime 2}} \frac{\Im m \mathcal{A}\left(\nu^{\prime}, t, Q^{2}\right)}{\nu^{\prime 2}-\nu^{2}}+\Delta\left(t, Q^{2}\right) \tag{3.45}
\end{equation*}
$$

where $\Delta\left(t, Q^{2}\right)$ is a possible subtraction that can be identified with the $D$-form factor 587. In combination with the leading order (LO) factorization (3.42), this implies for GPDs

$$
\begin{equation*}
\Re e \mathcal{A}\left(\xi, t, Q^{2}\right) \sim \int_{-1}^{1} d x \frac{G P D^{(+)}\left(x, \xi, t, Q^{2}\right)}{x-\xi}=\int_{-1}^{1} d x \frac{G P D^{(+)}\left(x, x, t, Q^{2}\right)}{x-\xi}+\Delta\left(t, Q^{2}\right) . \tag{3.46}
\end{equation*}
$$

Although its derivation from dispersion relations is more physical, (3.46) was first derived from polynomiality [574].

One of the consequences of (3.46) is that it allows to '"condense" the information from the DVCS amplitude (including the real part) into GPDs along the diagonal $x=\xi$ plus the D-form factor. However, it should be emphasized that this does not render measurements of the real part of the DVCS amplitude redundant. Indeed, measurements of $\Im m \mathcal{A}_{\text {DVCS }}$ for a given beam energy do not cover the whole region $0<\xi<1$ that enters (3.46). This implies that one can, for example, use $\Re e \mathcal{A}\left(\xi, t, Q^{2}\right)$ at fixed $Q^{2}$ to constrain $\operatorname{GPD}\left(\xi, \xi, t, Q^{2}\right)$ for the values of $\xi$ that are not accessible directly through the measurement of $\Im m \mathcal{A}\left(\xi, t, Q^{2}\right)$. In summary, a DVCS experiment at fixed $Q^{2}$ (large enough for GPD factorization to hold) should in principle allow for the determination of GPDs along the diagonal $x=\xi$ as well as the D-form factor, which (through the polynomiality condition) impose some constraints on GPDs for $x \neq \xi$.

Additional important constraints on GPDs come from their QCD evolution. The $Q^{2}$ evolution equations can be "diagonalized" by expanding GPDs in terms of Gegenbauer polynomials $C_{n}^{3 / 2}(x)$ :

$$
\begin{equation*}
G P D\left(x, \xi, t, Q^{2}\right)=\left(1-x^{2}\right) \sum_{n=0}^{\infty} C_{n}^{3 / 2}(x) \sum_{m=0(\text { even })}^{n} a_{n m}(\xi) \mathcal{C}_{n-m}\left(\xi, t, Q^{2}\right), \tag{3.47}
\end{equation*}
$$

where $a_{n m}(\xi)$ are known polynomials. The coefficients $\mathcal{C}_{k}\left(\xi, t, Q^{2}\right)$ are a priori unknown, but their $Q^{2}$ evolution is known. This allows one (in principle) to determine $\mathcal{C}_{k}\left(\xi, t, Q^{2}\right)$ model independently. For this purpose, let us consider $x=\xi$, where GPDs can be measured directly. Upon relabeling $k=n-m$, (3.47) reads

$$
\begin{equation*}
\operatorname{GPD}\left(\xi, \xi, t, Q^{2}\right)=\left(1-\xi^{2}\right) \sum_{k=0}^{\infty} \mathcal{C}_{k}\left(\xi, t, Q^{2}\right) f_{k}(\xi), \tag{3.48}
\end{equation*}
$$

where $f_{k}(\xi)=\sum_{m=0(\text { even })}^{\infty} a_{m+k, m}(\xi) C_{m+k}^{3 / 2}(\xi)$ are known functions. For any fixed $\xi$, each term in (3.48) evolves differently and, thus, a measurement over a wide range of $Q^{2}$ should allow for the determination of $\mathcal{C}_{k}\left(\xi, t, Q^{2}\right)$ as well as the GPDs for $x \neq \xi$ [via (3.47)]. At an EIC with its wide $Q^{2}$ range and high luminosity, it may be possible for the first time to carry out a model-independent extraction of GPDs. More detailed numerical studies will be required to quantify this expectation.

### 3.8 Accessing GPDs from experiment: potential of a highluminosity EIC

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### 3.8.1 Introduction

Generalized parton distributions (GPDs) [567, 568, 569] have received much attention from both the theoretical and experimental sides. This was triggered by the hope to solve the "spin puzzle" that refers to the mismatch between the quark contribution to the proton spin extracted from polarized DIS and the one given by the constituent quark model. We view the "spin puzzle" first and foremost as a quest to quantify the partonic structure of the nucleon in terms of quark and gluon angular momenta [274]. Furthermore, it has been realized that GPDs allow for a three-dimensional imaging of nucleons and nuclei 623], providing, in the zero-skewness case $(\xi=0)$, a probabilistic interpretation in terms of partonic degrees of freedom [579]. In fact, GPDs build up a whole framework for description of hadron structure [575, 576], with the "spin puzzle" being just one interesting aspect.

In phenomenology, GPDs are used for modeling elastic form factors and the description of hard exclusive leptoproduction and even photoproduction. For hard exclusive processes, factorization theorems have been proven in the collinear framework at twist-two level [572, 624. In the last decade, various hard exclusive processes have been measured by the H1 and ZEUS collaborations (DESY) in the small $x_{B}$ region and by HERMES (DESY), CLAS (JLAB), and Hall A (JLAB) in the moderate $x_{B}$ region in the fixed-target experiments.

Deeply virtual Compton scattering (DVCS) off nucleon is considered as the theoretically cleanest process offering access to GPDs. Its amplitude can be parameterized by twelve Compton form factors (CFFs) [625], which are given in terms of twist-two (including gluon transversity) and twist-three GPDs. For instance, at leading order (LO), parity-even twisttwo CFFs, $\mathcal{H}$ and $\mathcal{E}$, can be expressed through quark GPDs $H$ and $E$ :

$$
\left\{\begin{array}{c}
\mathcal{H}  \tag{3.49}\\
\mathcal{E}
\end{array}\right\}\left(x_{B}, t, \mathcal{Q}^{2}\right) \stackrel{\text { LO }}{=} \int_{-1}^{1} d x \frac{2 x}{\xi^{2}-x^{2}-i \epsilon}\left\{\begin{array}{l}
H \\
E
\end{array}\right\}\left(x, \eta=\xi, t, \mathcal{Q}^{2}\right),
$$

where both quark and anti-quark GPDs are defined in the region $x \in[-\xi, 1] ; x_{B}=$ $2 \xi /(1+\xi)$. Similar expressions can be written for twist-two parity-odd CFFs $\widetilde{\mathcal{H}}$ and $\widetilde{\mathcal{E}}$, while for other CFFs they are a bit more intricate 625]. Analogous formulae hold for the LO description of $\gamma^{*} N \rightarrow M N$ transition form factors (TFFs), measurable in deeply virtual electroproduction of mesons (DVEM). Here, in addition to GPDs, the non-perturbative meson distribution amplitude enters, which describes the transition of a quark-antiquark state into the final meson. This induces an additional uncertainty in the GPD phenomenology.

Let us briefly clarify which GPD information can be extracted from experimental measurements. Neglecting radiative and higher twist-contributions, one might view the GPD on the $\eta=x$ cross-over line as a "spectral function", which provides also the real part of the CFF via the "dispersion relation" [626, 627, 628, 629]:

$$
\begin{array}{rll}
\Im \mathrm{m} \mathcal{F}\left(x_{B}, t, \mathcal{Q}^{2}\right) & \stackrel{\mathrm{LO}}{=} \pi F\left(\xi, \xi, t, \mathcal{Q}^{2}\right), \quad F=\{H, E, \widetilde{H}, \widetilde{E}\}, \\
\Re \mathrm{e}\left\{\begin{array}{c}
\mathcal{H} \\
\mathcal{E}
\end{array}\right\}\left(x_{B}, t, \mathcal{Q}^{2}\right) & \stackrel{\mathrm{LO}}{=} \mathrm{PV} \int_{0}^{1} d x \frac{2 x}{\xi^{2}-x^{2}}\left\{\begin{array}{c}
H \\
E
\end{array}\right\}\left(x, x, t, \mathcal{Q}^{2}\right) \pm \mathcal{D}\left(t, \mathcal{Q}^{2}\right) . \tag{3.51}
\end{array}
$$

The GPD support properties ensure that (3.50) and (3.51) are in one-to-one correspondence to the perturbative formula (3.49), where the subtraction constant $\mathcal{D}$, which is related in a specific GPD representation to the so-called $D$-term [587], can be calculated from either $H$ or $E$. However, we note that the "dispersion relation" (3.51) is given in terms of partonic variables and compared to the dispersion relation formulated in physical variables it differs by power suppressed contributions. To pin down the GPD in the outer region $y \geq \eta=x$, one might employ evolution. For instance, in the non-singlet case, the change of the GPD on the cross-over line is governed by (the equation in the whole outer region is needed)

$$
\begin{equation*}
\mu^{2} \frac{d}{d \mu^{2}} F\left(x, x, t, \mu^{2}\right)=\int_{x}^{1} \frac{d y}{x} V\left(1, y / x, \alpha_{s}(\mu)\right) F\left(y, x, t, \mu^{2}\right) \tag{3.52}
\end{equation*}
$$

where $V$ is the evolution kernel [567]. Unfortunately, a large enough $\mathcal{Q}^{2}$ range is not available in fixed target experiments. Hence, we must conclude that in such measurements, essentially only the GPD on the cross-over line [thanks to (3.51), also outside of the experimentally accessible part of this line [629]] and the subtraction constant $\mathcal{D}$ can be accessed. Moments, such as those entering the spin sum rule, can only be obtained from a GPD model, fitted to data, or more generally with help of some "holographic" mapping [629]:

$$
\begin{equation*}
\left\{F\left(x, \eta=0, t, Q^{2}\right), F\left(x, \eta=x, t, Q^{2}\right)\right\} \quad \Longrightarrow \quad F\left(x, \eta, t, Q^{2}\right) . \tag{3.53}
\end{equation*}
$$

Here, $F\left(x, \eta=0, t, \mathcal{Q}^{2}\right)$ are constrained from form factor measurements and, additionally, GPDs $\widetilde{H}(H)$ by (un)polarized phenomenological PDFs. Of course, a given 'holographic' mapping holds only for a specific class of GPD models.

### 3.8.2 GPD modeling

The implementation of radiative corrections, even including LO evolution (3.52), requires to model CFFs or TFFs in terms of GPDs. This can be done in different representations, which should be finally considered as equivalent. However, for a specific purpose a particular representation may be more suitable than the others.

Neglecting positivity constraints, we model GPDs by means of a conformal SL( $2, \mathbb{R}$ ) partial wave expansion, which can be written as a Mellin-Barnes integral [630]:

$$
\begin{equation*}
F\left(x, \eta, t, \mu^{2}\right)=\frac{i}{2} \int_{c-i \infty}^{c+i \infty} d j \frac{p_{j}(x, \eta)}{\sin (\pi j)} F_{j}\left(\eta, t, \mu^{2}\right) \tag{3.54}
\end{equation*}
$$

Here, $p_{j}(x, \eta)$ are the partial waves given in terms of associated Legendre functions of the first and second kind, and the integral conformal GPD moments $F_{j}\left(\eta, t, \mu^{2}\right)$ are even polynomials in $\eta$ of order $j$ or $j+1$. Other representations of GPDs based on the $\operatorname{SL}(2, \mathbb{R})$ partial wave expansion include the so-called "dual" parameterization [631, 632, 633, 634].

In the Mellin-Barnes representation, the CFFs possess a rather convenient form, e.g., (3.49) can be rewritten in the following form [627, 635]:

$$
\begin{align*}
\left\{\begin{array}{c}
\mathcal{H} \\
\mathcal{E}
\end{array}\right\}\left(x_{B}, t, Q^{2}\right) \stackrel{\text { LO }}{=} & \frac{1}{2 i} \int_{c-i \infty}^{c+i \infty} d j \xi^{-j-1}\left[i+\tan \left(\frac{\pi j}{2}\right)\right] \\
& \times\left.\frac{2^{j+1} \Gamma(j+5 / 2)}{\Gamma(3 / 2) \Gamma(j+3)}\left\{\begin{array}{c}
H_{j} \\
E_{j}
\end{array}\right\}\left(\eta=\xi, t, Q^{2}\right)\right|_{\xi=\frac{x_{B}}{2-x_{B}}} . \tag{3.55}
\end{align*}
$$

This integral is numerically implemented in an efficient routine in two different factorization schemes, including the standard minimal subtraction ( $\overline{\mathrm{MS}}$ ) one at next-to-leading order (NLO) accuracy. Further advantages of this representation are:
(i) The conformal moments evolve autonomously at LO.
(ii) One can employ conformal symmetry to obtain next-to-next-to-leading order (NNLO) corrections to the DVCS amplitude 635, 636.
(iii) PDF and form factor constraints can be straightforwardly implemented. Namely, $F_{j}\left(\eta=0, t=0, \mu^{2}\right)$ are the Mellin moments of PDFs, $F_{j=0}$ are partonic contributions to elastic form factors, $H_{j=1}$ and $E_{j=1}$ are the energy-momentum tensor form factors, and for general $j$ one immediately makes contact to lattice measurements.

To parameterize the degrees of freedom that can be accessed in hard exclusive reactions, one can expand the conformal moments in terms of $t$-channel $\mathrm{SO}(3)$ partial waves expressed in terms of the Wigner rotation matrices $\hat{d}_{j}(\eta)\left(\hat{d}_{j}(\eta=0)=1\right)$ 637. An effective GPD model at given input scale $Q_{0}^{2}$ is provided by taking into account three partial waves,

$$
\begin{equation*}
F_{j}(\eta, t)=\hat{d}_{j}(\eta) f_{j}^{j+1}(t)+\eta^{2} \hat{d}_{j-2}(\eta) f_{j}^{j-1}(t)+\eta^{4} \hat{d}_{j-4}(\eta) f_{j}^{j-3}(t) \tag{3.56}
\end{equation*}
$$

which is valid for integral $j \geq 4$. In the simplest version of such a model, one might introduce just two additional parameters by setting the non-leading partial wave amplitudes to:

$$
\begin{equation*}
f_{j}^{j-k}(\eta, t)=s_{k} f_{j}^{j+1}(\eta, t), \quad k=2,4, \ldots . \tag{3.57}
\end{equation*}
$$

Such a model allows us to control the size of the GPD on the cross-over line and its $Q^{2}$ evolution, see fig. 3.28. A flexible parameterization of the skewness effect in the large $x$ region requires to decorate the skewness parameters $s_{k}$ with some $j$ dependence and for more convenience one might replace Wigner's rotation matrices by some effective $\mathrm{SO}(3)$ partial waves.

### 3.8.3 GPDs from hard exclusive measurements

Based on the experimental data set from the collider experiments H1 and ZEUS at DESY, the fixed target experiment HERMES at DESY, and the Hall A, CLAS, and Hall C experiments at JLAB, GPDs have been accessed from hard exclusive meson and photon electroproduction in the last few years. Favorably, DVCS enters as a subprocess into the hard photon electroproduction where its interference with the Bethe-Heitler (BH) bremsstrahlung process provides variety of handles on the real and imaginary part of twist-two and twistthree CFFs [625, 638]. However, switching from a proton to a neutron target allows only for a partial flavor separation, which is much more intricate than in DIS. On the other hand, DVEM can be used as a flavor filter, however, here one expects that both radiative 639, 640, 641 and (non-factorizable) higher-twist contributions might be rather important. The onset of the collinear description remains here an issue which should be explored.

For the DVCS process, the collinear factorization approach has been employed in a specific scheme up to NNLO in the small $x_{B}$ region 627, 635, 636]. It turns out that NLO corrections are moderate, while NNLO ones are becoming much smaller 627. Experimentally, the unpolarized DVCS cross section has been provided by the H1 and ZEUS collaborations [642, 643, 644, 645]. In the collider kinematics, the DVCS cross section is primarily given in terms of two CFFs, $\mathcal{H}$ and $\mathcal{E}$ :

$$
\begin{equation*}
\left.\frac{d \sigma^{\mathrm{DVCS}}}{d t}\left(W, t, Q^{2}\right) \approx \frac{\pi \alpha^{2}}{\mathcal{Q}^{4}} \frac{W^{2} x_{B}^{2}}{W^{2}+Q^{2}}\left[|\mathcal{H}|^{2}-\frac{t}{4 M_{p}^{2}}|\mathcal{E}|^{2}\right]\left(x_{B}, t, \mathcal{Q}^{2}\right)\right|_{x_{B} \approx \frac{Q^{2}}{W^{2}+Q^{2}}} \tag{3.58}
\end{equation*}
$$



Figure 3.21. Quark (a) and gluon (b) transverse profile function (3.59) for $Q^{2}=4 \mathrm{GeV}^{2}$ and $x=10^{-3}$ from a six parameter DVCS fit 646.

Although at a fixed scale and to LO accuracy the CFFs are given by (dominant sea) quark GPDs, evolution will induce a gluonic contribution, too. Indeed, the experimental lever arm $3 \mathrm{GeV}^{2} \lesssim Q^{2} \lesssim 80 \mathrm{GeV}^{2}$ is sufficiently large to access the gluonic GPD. In our fitting procedure, the Mellin-Barnes integral was utilized within a $\mathrm{SO}(3)$ partial wave ansatz for the conformal moments and good fits ( $\chi^{2} /$ d.o.f. $\approx 1$ ) could be obtained at LO to NNLO accuracy, exemplifying that flexible GPD models were at hand. From such fits, one can then obtain the image of quark and gluon distributions. It is illustrated in figure 3.21 that in impact space, the (normalized) transverse profiles,

$$
\begin{equation*}
\rho\left(b, x, Q^{2}\right)=\frac{\int_{-\infty}^{\infty} d^{2} \vec{\Delta} e^{i \vec{\Delta} \vec{b}} H\left(x, \eta=0, t=-\vec{\Delta}^{2}, Q^{2}\right)}{\int_{-\infty}^{\infty} d^{2} \vec{\Delta} H\left(x, \eta=0, t=-\vec{\Delta}^{2}, Q^{2}\right)}, \tag{3.59}
\end{equation*}
$$

determined for dipole and exponential $t$-dependence of $H$, mainly differ for distances larger than the disc radius of the proton, i.e., for $b>0.6 \mathrm{fm}$. Hence, the larger values of the transverse widths, $\sqrt{\left\langle\vec{b}^{2}\right\rangle}{ }_{\text {sea }} \approx 0.9 \mathrm{fm}$ and $\sqrt{\left\langle\vec{b}^{2}\right\rangle} \approx 0.8 \mathrm{fm}$ for the dipole ansatz, arise from the long-range tail of the profile function, see the solid curves in figure 3.21 For an exponential ansatz, we find slightly smaller values $\sqrt{\left\langle\vec{b}^{2}\right\rangle}$ sea $\approx 0.7 \mathrm{fm}$ and $\sqrt{\left\langle\overrightarrow{b^{2}}\right\rangle}{ }_{\mathrm{G}} \approx 0.6 \mathrm{fm}$, where the gluonic one is compatible with the analysis of $J / \psi$ production [594]. Note that the model uncertainty in the extrapolation of the GPD to $t=0$ corresponds to the uncertainty in the long-range tail. Moreover, the model uncertainty of the extrapolation into the region $-t>1 \mathrm{GeV}^{2}$ is essentially canceled in the profile (3.59) normalized at $b=0$.

We also note that at LO the gluonic GPD (as the gluonic PDF) is rather steep and radiative corrections might provide a large GPD/PDF reparameterization effect, which will be studied in more detail in the future. Our first successful LO description of DVCS within a flexible GPD model [646] is in agreement with aligned-jet model considerations 647]. We also mention that an attempt has been undertaken to access the $\mathcal{E}$ CFF from the beam charge asymmetry measurement [648], proportional to the combination $\Re \mathrm{e}\left[F_{1}(t) \mathcal{H}-\frac{t}{4 M^{2}} F_{2}(t) \mathcal{E}\right]$. Unfortunately, the size of the experimental uncertainties does not allow one to separate the $\mathcal{H}$ and $\mathcal{E}$ contributions.

An approach analogous to the one employed for DVCS [627] is also suitable for LO and NLO analysis of DVEM. Hence, one can simultaneously make use of DVCS and DVEM measurements in a global fitting procedure, which is in progress.

GPD studies were also performed for the DVCS process in the fixed target kinematics
to LO accuracy. In this region, relying on the scaling hypothesis, one might directly ask for the value of the GPDs on their cross-over line. For instance, for valence quarks we use the following generically motivated ansatz:

$$
\begin{equation*}
H^{\mathrm{val}}(x, x, t)=\frac{1.35 r}{1+x}\left(\frac{2 x}{1+x}\right)^{-\alpha(t)}\left(\frac{1-x}{1+x}\right)^{b}\left(1-\frac{1-x}{1+x} \frac{t}{M^{\mathrm{val}}}\right)^{-1} \tag{3.60}
\end{equation*}
$$

where $r=\lim _{x \rightarrow 0} H(x, x) / H(x, 0)$ is the skewness ratio; $\alpha(t)=0.43+0.85 t / \mathrm{GeV}^{2} ; b$ controls the $x \rightarrow 1$ limit and $M^{\text {val }}$ controls the residual $t$-dependence, which we set to $M^{\mathrm{val}}=0.8 \mathrm{GeV}$. For the forward limit $q(x)=H(x, 0)$, we used the LO parameterization of Alekhin [649]. The generic $(-t)^{-2}$ fall-off at large $-t$ for generalized form factors is indirectly encoded in the Regge-trajectory and the residual $t$ dependence is modeled by a monopole form with an $x$-dependent cut-off mass. The subtraction constant (3.51) is taken an a dipole form:

$$
\begin{equation*}
\mathcal{D}(t)=d\left(1-\frac{t}{M_{d}^{2}}\right)^{-2} . \tag{3.61}
\end{equation*}
$$

In a first global fit 646] to hard exclusive photon electroproduction off unpolarized proton, we took sea quark and gluon GPD models with two $\mathrm{SO}(3)$ partial waves at small $x$, reparameterized the outcome from H1 and ZEUS DVCS fits at $Q^{2}=2 \mathrm{GeV}^{2}$, and employed it in fits of fixed target data within the scaling hypothesis. To relate the CFFs with the observables, we employed the BKM formulas 625 within the 'hot-fix' convention 650 and used the Sachs parameterization for the electromagnetic form factors. Thereby, we utilized the "dispersion relation" (3.50]3.51), where the ansatz (3.60) specifies a valence-like GPD on the cross-over line. Besides the subtraction constant (3.61), we also included the parameterfree pion-pole model for the $\tilde{E}$ GPD 651 and parameterized the $\widetilde{H}$ GPD rather analogously to (3.60) with $b=3 / 2$. For the fixed target fits, we chose two data sets resulting in two fits (KM09a and KM09b). Out fit gives:

$$
\begin{array}{lllll}
\text { KM09a: } & b^{\text {sea }}=3.09, & r^{\mathrm{val}}=0.95, \quad b^{\mathrm{val}}=0.45, & d=-0.24, & M_{d}=0.5 \mathrm{GeV}, \\
\text { KM09b: } & b^{\text {sea }}=4.60, \quad r^{\mathrm{val}}=1.11, \quad b^{\mathrm{val}}=2.40, & d=-6.00, & M_{d}=1.5 \mathrm{GeV}(.3 .62)
\end{array}
$$

These values of the fit parameters are compatible with our generic expectations: the skewness effect at small $x$ should be small, i.e., $r \sim 1$, the subtraction constant should be negative [574, 652, and, according to counting rules 653], $b$ should be smaller than the corresponding $\beta$ value of the relevant PDF [646, 654].

To improve the models that we just described, we now use a hybrid technique where the sea quark and gluon GPDs are represented in terms of conformal moments, while, for convenience, the valence quarks are still modeled in momentum fraction space and within the "dispersion integral" approach. Also, the residue of the pion-pole contribution is now considered as a parameter, and the Hall A data forces a roughly three times larger value than expected from the model 651]. Optionally, we might also use the improved formulae from [655] applicable for a longitudinally polarized target. The new parameters read:

$$
\begin{array}{ll}
\text { KM10a: } & r^{\mathrm{val}}=0.88, \quad M^{\mathrm{val}}=1.5 \mathrm{GeV}, \quad b^{\mathrm{val}}=0.40, d=-1.72, \quad M_{d}=2.0 \mathrm{GeV}, \\
\text { KM10b: } & r^{\mathrm{val}}=0.81, \quad M^{\text {val }}=0.8 \mathrm{GeV}, \quad b^{\mathrm{val}}=0.77, \quad d=-5.43, \quad M_{d}=1.33 \mathrm{Ge(B.63)}
\end{array}
$$

Note that for the valence part of the $H$ GPD, these results are qualitatively compatible with those from the pure KM09 "dispersion relation" fits.


Figure 3.22. Experimental measurements for fixed target kinematics (circles) labeled by data point number $n$ : $A_{\mathrm{BS}}^{(1)}(1-18), A_{\mathrm{BC}}^{(0)}(19-36), A_{\mathrm{BC}}^{(1)}(37-54)$ from [656]; $A_{\mathrm{BS}}^{(1)}(55-66)$ and $\Sigma_{\mathrm{BS}}^{(1), w}(67-70)$ are derived from 657] and 658. Model results are from the "dispersion-relation" fits KMO9a without Hall A data 646 (squares, slightly shifted to the left) and KMO9b with the Hall A data (circles, slightly shifted to the right), hybrid model fit KM10b (triangles-up), and a hand-bag prediction GK07 from hard vector meson production (triangles-down, slightly shifted to the r.h.s.) [659].

We also performed an additional fit where we directly used the harmonics of beam spin sums and differences measured by Hall A (fit KM10). The results of our two "dispersionrelation" fits and three hybrid model fits are available as a computer program providing the four-fold cross section of polarized lepton scattering on unpolarized proton for a given kinematics, see http://calculon.phy.hr/gpd/. Unlike "dispersion-relation" fits, the hybrid model fits, where LO evolution of sea quark and gluon GPDs has been taken into account, are suitable for estimates in the small $x_{B}$ region.

In figure 3.22 we confront our fit results $\left(\chi^{2} /\right.$ d.o.f. $\approx 1$ w.r.t. the employed data sets) to experimental data: KM09a (squares), KM09b (circles), and the hybrid model fit KM10b (triangles-up) in which we now utilized the improved formulae set 655 and the Kelly form factor parameterization 660]. We also include the predictions from the GK07 model [659] (triangles-down), where we adopt the hypothesis of $H$ dominance. Qualitatively, these predictions are consistent with a $\mathrm{VGG}^{2}$ code estimate, which tends to over-estimate the BSAs [657, 656] and describes the BCAs from HERMES rather well without the $D$-term [661]. This is perhaps not astonishing, since the employed $H$ GPD model relies on Radyushkin's DD ansatz, too. We would like to emphasize that at LO, the GK07 model is in reasonable agreement with the H1 and ZEUS DVCS data $\left(\chi^{2} /\right.$ d.o.f. $\left.\approx 2\right)$, essentially thanks to the rather small and stable skewness ratio $r^{\text {sea }}$ of sea quarks.

Longitudinally polarized target data from CLAS 662 and HERMES 663 provide a handle on $\widetilde{H}$ 625, where the mean values of CFF fits 664 in the JLAB kinematics give two to three times bigger $\widetilde{H}$ contribution compared to our expectations $\left(r_{\widetilde{H}} \simeq 1, b_{\widetilde{H}} \simeq 2\right)$. These findings are one to two standard deviations away from our big $\widetilde{H}$ ad hoc scenario of the KM09b fit, which is indeed disfavored by the longitudinally polarized proton data. We like to add that with our present hybrid model a reasonable global fit, such as KM10 above, is possible. In such a fit, the Hall A data require a rather large pion pole contribution, inducing a large DVCS cross section contribution. Still, we have not included the transversal

[^272]

Figure 3.23. $\Im m \mathcal{H} / \pi$ from different strategies: our DVCS fits [dashed (solid) curve excludes (includes) Hall A data from "dispersion relation" KM09a (KM09b) 646 and hybrid KM10b (dashdotted) models], GK07 model from DVEM (dotted), seven-fold CFF fit 666, 667 with boundary conditions (squares), $\mathcal{H}, \widetilde{\mathcal{H}} \mathrm{CFF}$ fit 664 (diamonds), smeared conformal partial wave model fit 668] within $H$ GPD (circles). The triangles result from our neural network fit, cf. figure 3.24.
target data from the HERMES collaboration [661] or the neutron data from Hall A 665].
So far we did not study model uncertainties or experimental error propagation, since both tasks might be rather intricate. To illuminate this, in figure 3.23 we compare our results for $\Im m \mathcal{H}\left(x_{B}, t\right) / \pi$ with the results that do provide error estimates. The squares arise from constrained least squares fits [666, 667] at given kinematic means of HERMES and JLAB measurements on unpolarized proton, where the imaginary and real parts of twist-two CFFs are taken as parameters. The huge size of the error bars shows the limited accuracy with which $H$ can be extracted from unpolarized proton data alone 625]. A pure $H$ GPD model fit 668] (circles) to JLAB data provides much smaller errors, arising from error propagation and some estimated model uncertainties. All three of our curves are compatible with the findings [666, 667] and the $H$ GPD model analysis [668] of CLAS data. However, for Hall A kinematics, the deviation of the two predictions that are based on the $H$ dominance hypothesis (the dashed curve and circles in the right panel) are obvious and are explained by our underestimation of the cross section normalization by about $50 \%$. Moreover, the quality of fit [668, $\chi^{2} /$ d.o.f. $\sim 1.7$, might provide another indication that CLAS and Hall A data are not compatible, when this hypothesis is assumed, see, e.g., the two rightmost circles in the left panel for CLAS ( $x_{B}=0.34, t=-0.3 \mathrm{GeV}^{2}, Q^{2}=2.3$ $\left.\mathrm{GeV}^{2}\right)$ and Hall $\mathrm{A}\left(x_{\mathrm{Bj}}=0.36, t=-0.28 \mathrm{GeV}^{2}, Q^{2}=2.3 \mathrm{GeV}^{2}\right)$. While the pure $\mathcal{H}$ and $\widetilde{\mathcal{H}}$ CFF fit 664 (diamonds), including longitudinally polarized target data, is within error bars inconsistent with the $H$ dominated scenario [668] (circles), it (accidentally) reproduces our dashed curve.

Another source of uncertainties are twist-three contributions and perhaps also gluon transversity related contributions, which might be strongly affected by twist-four effects [669].

All this exemplifies that within (strong) assumptions and the present set of measurements, the propagated experimental errors cannot be taken as an estimate of GPD uncertainties. An error estimation in model fits might be based on twist-two sector projection technique [625], boundaries for the unconstrained model degrees of freedom, and error propagation in the twist-two sector. Alternatively, neural networks, already successfully used for PDF fits [47, may be an ideal tool to extract CFFs or GPDs. In figure 3.24, we present a first example in which, within the $H$-dominance hypothesis, $\mathcal{H}$ is extracted using a pro-


Figure 3.24. Neural network extraction of $\Re \mathrm{e} \mathcal{H}\left(x_{B}, t\right) / \pi$ from BCA 656] and BSA 657] data.
cedure similar to the one of 670. Here, 50 feed-forward neural nets with two hidden layers were trained using HERMES BCA [656] and CLAS BSA 657] data. Hence, only the experimental errors were propagated, which, in the absence of a model hypothesis, become large for the $t \rightarrow 0$ extrapolation.

### 3.8.4 Potential of an electron-ion collider

A high luminosity machine in the collider mode with polarized electron and proton or ion beams would be an ideal instrument to quantify QCD phenomena. It is expected that such a machine, combined with designated detectors, would allow for precise measurements of exclusive channels. Besides hard exclusive vector meson and photon electroproduction, one might address the behavior of parity-odd GPDs $\widetilde{\mathcal{H}}$ (related to polarized PDFs) and $\widetilde{\mathcal{E}}$ via the exclusive production of pions even in the small $x$ region. It is obvious from what was said above that an access of GPDs requires a large data set with small errors. In the following we would like to illustrate the potential of such a machine for DVCS studies, where we also address the GPD deconvolution problem.

Let us remind that already the isolation of CFFs is rather intricate. For a spin- $1 / 2$ target, we have four twist-two, four twist-three, and four gluon transversity-related complex valued CFFs. The photon helicity non-flip amplitudes are dominated by twist-two CFFs, the transverse-longitudinal flip amplitudes by twist-three effects, and the transverse-transverse flip ones by gluon transversity. Hence, the first, second, and third harmonics w.r.t. the azimuthal angle of the interference term are twist-two, twist-three, and gluon transversity dominated, respectively. In an ideal experiment, assuming that transverse photon helicity flip effects are negligible, cross section measurements would allow to separate the sixteen quantities that are then given in terms of twist-two and twist-three CFFs. The reader might find a more detailed discussion, based on a $1 / Q$ expansion, in 625. We also note that the definition of CFFs is convention-dependent.

In a twist-two analyzes on unpolarized, longitudinally and transversally polarized protons, one might be able to disentangle the four different twist-two CFFs via the measurement of single beam and target spin asymmetries. In figure 3.25, we illustrate that the beam spin asymmetry for a proton target (solid curves),

$$
\begin{equation*}
A_{\mathrm{BS}}^{(1)} \propto \frac{\sqrt{t_{\min }-t}}{2 M} y\left[F_{1}(t) H\left(\xi, \xi, t, Q^{2}\right)-\frac{t}{4 M^{2}} F_{2}(t) E\left(\xi, \xi, t, Q^{2}\right)+\cdots\right], \tag{3.64}
\end{equation*}
$$



Figure 3.25. KM10b model estimate for the DVCS beam spin asymmetry with a proton (solid) and neutron (dashed) target. Left panel: $A_{\mathrm{BS}}$ vs. $\phi$ for $E_{N}=250 \mathrm{GeV}, E_{e}=5 \mathrm{GeV}, x_{B}=5 \times 10^{-3}$, $Q^{2}=10 \mathrm{GeV}^{2}$, and $t=-0.2 \mathrm{GeV}^{2}$. Right panel: Amplitude $A_{\mathrm{BS}}^{(1)}$ of the first harmonic vs. $x_{\mathrm{Bj}}$ at $t=-0.2 \mathrm{GeV}^{2}$ for small $x_{B}$ (thin) $\left[E_{e}=30 \mathrm{GeV}, E_{p}=360 \mathrm{GeV}, Q^{2}=4 \mathrm{GeV}^{2}\right]$ and large $x_{B}$ (thick) $\left[E_{e}=5 \mathrm{GeV}, E_{p}=150 \mathrm{GeV}, Q^{2}=50 \mathrm{GeV}^{2}\right]$ kinematics.
might be rather sizeable over a large kinematical region in which the lepton energy loss $y$ is not too small. Here the helicity conserved CFF $\mathcal{H}$ is the dominant contribution, while $\mathcal{E}$ appears with a kinematic suppression factor $t / 4 M^{2}$, induced by the helicity flip. For a neutron target, the $\mathcal{H}$ contribution is suppressed by the accompanying Dirac form factor $F_{1}^{n}$ $\left(F_{1}^{n}(t=0)=0\right)$ and, hence, one becomes sensitive to the CFF $\mathcal{E}$. Unfortunately, one also has to worry about other non-dominant CFF contributions, indicated by the ellipsis. Note that the asymmetry for the neutron (dashed curves in figure 3.25) might be underestimated since we set in our model $E\left(x, x, t, Q^{2}\right)$ to zero.

For a longitudinally polarized target, the asymmetry

$$
\begin{equation*}
A_{\mathrm{TS}}^{\Rightarrow(1)} \propto \frac{\sqrt{t_{\mathrm{min}}-t}}{2 M}\left[F_{1}(t) \widetilde{H}\left(\xi, \xi, t, \mathcal{Q}^{2}\right)-\frac{t}{4 M^{2}} F_{2}(t) \xi \widetilde{E}\left(\xi, \xi, t, \mathcal{Q}^{2}\right)+\cdots\right] \tag{3.65}
\end{equation*}
$$

is sensitive to the GPD $\widetilde{H}$, while $\xi \widetilde{E}$ and other GPDs might contribute to some extent. Naively, one would expect that this asymmetry vanishes in the small $x_{B}$ region and might be sizeable at $x_{B} \sim 0.1$, see the left panel of figure 3.26 . Not much is known about the small $x$ behavior of $\widetilde{H}$ and it might be even accessible at smaller values of $x_{B}$, as illustrated by the $K M 09 b$ model with its big $\widetilde{H}$ contribution (solid curve, the right panel of figure 3.26 ). For a neutron target, the asymmetry becomes sensitive to the $\xi \widetilde{E}$ GPD. Note that here the factor $\xi$ is annulled by a conventional $1 / \xi$ factor in the definition of the $\widetilde{E}$ GPD.

Finally, we emphasize that a single spin asymmetry measurement with a transversally polarized target provides another handle on the helicity-flip GPDs $E$ and $\widetilde{E}$. If the target spin is perpendicular to the reaction plane, the asymmetry

$$
\begin{equation*}
A_{\mathrm{TS}}^{\Uparrow(1)} \propto \frac{t}{4 M^{2}}\left[F_{2}(t) H\left(\xi, \xi, t, \mathcal{Q}^{2}\right)-F_{1}(t) E\left(\xi, \xi, t, \mathcal{Q}^{2}\right)+\cdots\right] \tag{3.66}
\end{equation*}
$$

is dominated by a linear combination of the GPDs $H$ and $E$. In the case when the target spin is aligned with the reaction plane, the asymmetry

$$
\begin{equation*}
A_{\mathrm{TS}}^{\Downarrow(1)} \propto \frac{t}{4 M^{2}}\left[F_{2}(t) \widetilde{H}\left(\xi, \xi, t, \mathcal{Q}^{2}\right)-F_{1}(t) \xi \widetilde{E}\left(\xi, \xi, t, \mathcal{Q}^{2}\right)+\cdots\right] \tag{3.67}
\end{equation*}
$$



Figure 3.26. DVCS longitudinal target spin asymmetry vs. $\phi$ for KM09a (dashed), KM09b (solid), and KM10b hybrid (dash-dotted) models at $E_{e}=5 \mathrm{GeV}, t=-0.2 \mathrm{GeV}^{2}, \mathcal{Q}^{2}=4 \mathrm{GeV}^{2}$ within $E_{p}=150 \mathrm{GeV}, x_{\mathrm{Bj}}=0.1$ (left) and $E_{p}=350 \mathrm{GeV}, x_{\mathrm{Bj}}=0.01$ (right).

Unfortunately, compared to the single beam spin (3.64) and longitudinal target (3.65) asymmetries, the transversally ones are kinematically suppressed by an additional factor $\sim \sqrt{-t} /(2 M)$ and, for a neutron target, in addition by the Dirac form factor $F_{1}(t)$.

Although the given formulae (3.64 3.67) are rather crude, they illustrate that a measurement of single spin asymmetries would allow to access the imaginary part of the four twist-two related CFFs. However, the normalization of these asymmetries depends to some extent also on the real part of the twist-two related CFFs and the remaining eight ones. Measurements of cross section differences would allow one to eliminate the normalization uncertainty, and in combination with the harmonic analysis, one can separate to some extent twist-two, twist-three, and gluon transversity contributions. However, the extracted harmonics might also be contaminated by DVCS cross section contributions which are bilinear in the CFFs. To get rid of these admixtures, one needs cross section measurements with a positron beam. Forming differences and sums of cross section measurements with both kinds of leptons, allows one to extract the pure interference and DVCS squared terms and, thus, might allow one to quantify twist-three effects. Existing data indicate that these effects are small as expected based on kinematic factors. However, even obtaining only an upper limit is important for the determination of the systematic uncertainties of twist-two CFFs.

We also emphasize that having both kinds of lepton beams available allows one to measure the real part of CFFs. In figure 3.27, we show the beam charge asymmetry,

$$
\begin{equation*}
A_{\mathrm{BC}}^{(1)} \propto \Re \mathrm{e}\left[F_{1}(t) \mathcal{H}\left(x_{\mathrm{Bj}}, t, \mathcal{Q}^{2}\right)-\frac{t}{4 M^{2}} F_{2}(t) \mathcal{E}\left(x_{\mathrm{Bj}}, t, \mathcal{Q}^{2}\right)+\cdots\right], \tag{3.68}
\end{equation*}
$$

for an unpolarized target, which is expected to be sizeable. For a proton target, this asymmetry should possess a node in the transition from the valence to sea region(thick solid curve, right panel). In our parameterization, the real part of the $\mathcal{E}$ CFF is determined by the $\mathcal{D}$ subtraction term, which induces a sizeable asymmetry (thick dashed curve, right panel), even for a neutron target.

The large kinematical coverage of the proposed high-luminosity EIC raises the question: Can one utilize evolution, even at moderate $x_{B}$ values, to access GPDs away from their crossover line? Similarly to what has been done for the small $x_{B}$ region, we use the Mellin-Barnes integral technique to address the problem. Taking different non-leading SO(3) partial waves in the ansatz for the conformal moments (3.56[3.57), we build three different GPD models


Figure 3.27. KM10b model estimate for the DVCS beam charge asymmetry with a proton (solid) and neutron (dashed) target. Left panel: $A_{\mathrm{BC}} v s . \phi$ for $E_{N}=250 \mathrm{GeV}, E_{e}=5 \mathrm{GeV}, x_{B}=5 \times 10^{-3}$, $Q^{2}=10 \mathrm{GeV}^{2}$, and $t=-0.2 \mathrm{GeV}^{2}$. Right panel: Amplitude $A_{\mathrm{BC}}^{(1)}$ of the first harmonic vs. $x_{B}$ at $t=-0.2 \mathrm{GeV}^{2}$ for small $x_{B}$ (thin) $\left[E_{e}=30 \mathrm{GeV}, E_{p}=360 \mathrm{GeV}, Q^{2}=4 \mathrm{GeV}^{2}\right]$ and large $x_{B}$ (thick) $\left[E_{e}=5 \mathrm{GeV}, E_{p}=150 \mathrm{GeV}, Q^{2}=50 \mathrm{GeV}^{2}\right]$ kinematics.
for valence quarks that provide almost identical CFFs, see the upper left panel in figure 3.28 , They are compatible with (3.60) from the "dispersion-relation" fit KM09a (dotted curves). We note that the different model behavior at large $x_{B}$ results only in a small discrepancy for the real part of the CFF in the kinematics of interest. In the lower left panel of figure 3.28, we illustrate that for fixed $\eta$, the $x$-shape of the three GPD models looks quite differently. Compared to the minimalist model (dotted curve), a model with a negative next-to-leading partial wave (solid) decreases the size of the GPD on the cross-over line $\eta=x$ and generates an oscillating behavior in the central region. The model with an alternating-sign $\mathrm{SO}(3)$ partial wave expansion (dash-dotted) possesses more pronounced oscillation effects in the central region or even nodes. In the third model (dashed curve), the reduction on the cross-over line is reached within a next-to-next leading $\mathrm{SO}(3)$ partial wave. Note that the GPDs in the region $\eta \ll x$ are governed by the $x$-behavior of the PDF analogues. In the right panels, we demonstrate that for a large lever arm in $Q^{2}$ (e.g., $Q^{2}=50 \mathrm{GeV}^{2}$ ), the evolution effects are important in the valence quark region. However, for CFFs (the upper right panel), the discriminating power of evolution effects remains moderate even if the GPD shapes look rather different.

### 3.8.5 Conclusions and summary

With all the theoretical tools sketched above plus those which are presently under development, it is clear that our understanding of hadron structure will be revolutionized once most of the diverse asymmetries are measured with percent or permille precision (depending on the observable). At present, first steps have been undertaken to access GPDs from experimental data in the small $x_{B}$ region and in the fixed target kinematics providing us with some insight into the GPD $H$. In particular, for DVCS in the fixed target kinematics, LO model fits are compatible with least-square CFF fits and first results from neural networks (assuming $H$ dominance). The large uncertainties in extracting CFFs are mainly related to the lack of experimental data. Thus, not only the extraction of the very desired $\mathcal{E}$ playing an important role in the "spin-puzzle", but also of other CFFs, requires a comprehensive measurement of all possible observables in dedicated experiments. A further comparison


Figure 3.28. Upper left panel: The valence-like contribution (3.60) to the CFF $\mathcal{H}$ extracted with a "dispersion-relation" fit KM09a from fixed target measurements (dotted) at $t=-0.2 \mathrm{GeV}^{2}$ and $Q^{2}=2 \mathrm{GeV}^{2}$ vs. $x_{B}$ together with various models. Lower left panel: The corresponding models of the GPD $x H\left(x, \eta, t, \mathcal{Q}^{2}\right)$ together with a minimalist GPD parameterization (dotted curve) vs. $x$ at $\eta=0.2, t=-0.2 \mathrm{GeV}^{2}$, and $Q^{2}=2 \mathrm{GeV}^{2}$. The same quantities at $Q^{2}=50 \mathrm{GeV}^{2}$ are displayed in the right panels.
shows that while in the valence region the extracted quark GPDs are somewhat different, they become compatible for small $x$. The main difference lies in the gluonic sector; a more appropriate analysis requires the inclusion of radiative corrections in a global fitting procedure, which is in progress. We should also mention here that hard exclusive processes with nuclei, which at present are not extensively studied, open a new window for the partonic view of nuclei.

Imaging the partonic content of the nucleon and the phenomenological access to the proton spin sum rule from hard exclusive processes can only be reached through proper understanding of GPD models. We also point out that GPDs can also be formulated in terms of an effective nucleon (light-cone) wave function, which links GPDs to transverse momentum dependent parton distributions. The whole framework consisting of perturbative QCD, lattice simulations, and dynamical modeling is available to reveal GPDs and access the nucleon wave function. Such a unifying description can be considered as the primary goal in quantifying the partonic picture. While such a task looks rather straightforward, much effort is needed on the theoretical, phenomenological, and experimental sides, with experimental data with small uncertainties playing the key role. A high-luminosity EIC is an ideal machine that would cover a wide kinematical range and complement the planned fixed target experiments at JLab@12 GeV. Thus, besides new measurements, an EIC has a great potential to significantly improve existing data sets.
Acknowledgments. We are grateful to P. Kroll for many fruitful discussions.

### 3.9 Monte Carlo studies on DVCS with an EIC

Salvatore Fazio

### 3.9.1 Exclusive processes with a dedicated EIC detector

Our current knowledge of the role of gluons in hadronic matter comes mainly from DIS experiments of electrons off protons most notably from HERA at DESY. Although electrons only interact with electrically charged particles, and gluons carry only color charge, a highenergy electron beam can still be used as an excellent gluon microscope.

The HERA physics program of ep collisions surprisingly showed a large fraction of diffractive events contributing $10-15 \%$ to the total DIS cross-section. One of the key signatures of these "diffractive" events is an intact proton traveling at nearly beam energies, together with a gap in rapidity before some final-state particles are produced at mid-rapidity. However, the detectors (H1 and ZEUS) were not optimized for this important physics and were unable to measure the scattered proton; this was only achievable after a program of upgrades. In fact, to measure diffractive physics events, it is desirable to have very forward detectors at small angles with respect to the beam line, referred to as "Roman Pots". Other requirements are that the detector should be able to measure all processes: inclusive ( $e p \rightarrow e^{\prime} X$ ), semi-inclusive ( $e p \rightarrow e^{\prime} X+$ hadrons), and exclusive (e.g., $e p \rightarrow e^{\prime} p+J / \psi$ ) reactions. The requirements for $e p$ and $e A$ collisions are very similar, the only additional complication in $e A$ collisions arises from the need to tag the struck nucleus, or to veto events with the nucleus break-up by detecting neutrons and other breakup products with high efficiencies.

Briefly, a possible EIC detector consists (in the barrel region at mid-rapidity) of a solenoidal field with Si tracking with full rapidity coverage around the interaction point itself, followed by Cherenkov detectors for particle identification and then by both electromagnetic and hadronic calorimeters. There are further trackers and calorimeters at forward rapidities, but this time, the magnetic field is a dipole. A Roman Pots spectrometer can be installed along the beam-pipe in the direction of the outgoing proton. This is just a starting point and other technologies are under active investigation.

### 3.9.2 DVCS and GPDs: from HERA to an EIC

Measurements of observables associated with hard exclusive processes at an ep/eA collider requires substantially higher luminosities than traditional inclusive DIS because of the small cross sections and the need for differential measurements. The detectors and the interaction region have to be designed to permit full reconstruction of the final state.

In assessing the prospects for measurements of exclusive processes in ep scattering at collider energies, $W^{2} \gg 10 \mathrm{GeV}^{2}$, one needs to distinguish between "diffractive" (no exchange of quantum numbers between the target and the projectile/produced system) and "non-diffractive" processes (exchange of quantum numbers). In diffractive channels, such as $J / \psi, \rho, \phi$ production and DVCS (production of a real photon), the cross sections rapidly rise with the collision energy, $W$. At large $Q^{2}$, these processes probe the gluon GPD and/or the singlet quark GPD. In non-diffractive channels, such as $\pi^{ \pm}, \pi^{0}, \rho^{+}, K$ production, the cross sections decrease with energy. These processes at high $Q^{2}$ probe the flavor/charge/spin non-singlet quark GPDs describing the quark structure of the target.

The final state of a DVCS event, shown in figure 3.29a, contains one track and two


Figure 3.29. Diagram of the DVCS (a) and BH processes for a photon emitted from the initial (b) and final (c) lepton line.
electromagnetic clusters together with a proton scattered at a very small angle. The technique for measuring DVCS consists of first extracting a data sample of events characterized by the DVCS topology. Apart from the DVCS process, the data selection comprises also Bethe-Heitler (BH) events, a well known QED process, because DVCS and BH share the same final state. The selected sample will contain a mixture of DVCS and BH contributions. For not too large $y$ (see figure 3.31), the BH contribution is not much larger than DVCS and thus can be subtracted from the data using the MC predictions and control data samples containing BH only since at high enough $Q^{2}$ the interference contribution drops out to a good accuracy when averaging over the angle $\phi$ between the production and scattering planes.

The differential cross section as a function of $|t|$ can be parameterized by an exponential: $d \sigma / d t \propto e^{b|t|}$. The H1 Collaboration [648] measured $|t|$ from the transverse momentum distribution of the photon and studied the $b$-slope in a few bins in $Q^{2}$ and $W$. The slope $b$ seems to decrease with $Q^{2}$ up to the value expected for a hard process but it does not depend on $W$. The ZEUS Collaboration [645] performed a direct measurement of the proton final state using a Roman Pots spectrometer: the resulting $b=4.5 \pm 1.3 \pm 0.4 \mathrm{GeV}^{-2}$ at $Q^{2}=3.2 \mathrm{GeV}^{2}$ and $W=104 \mathrm{GeV}$ is consistent, within the large uncertainties due to the low acceptance of the spectrometer, with the H 1 result of $b=5.45 \pm 0.19 \pm 0.34 \mathrm{GeV}^{-2}$ at $Q^{2}=8 \mathrm{GeV}^{2}$ and $W=82 \mathrm{GeV}$ [648].

A comprehensive program of parton imaging in the nucleon would need precise measurements of $b$ for wide range of $x_{B}$ values, $10^{-4}<x_{B}<10^{-1}$; this is currently beyond the possibilities of any experiment. Building an EIC with a properly designed detector could finally make it possible - a preliminary feasibility study is reported in section 3.6.

The beam-charge asymmetry (BCA) provides an access to the real part of the DVCS amplitude through the interference between the DVCS and BH amplitudes (for illustration, we keep only the dominant $\cos (\phi)$ harmonic):

$$
\begin{equation*}
A_{C}=\frac{\frac{d \sigma^{+}}{||t|}-\frac{d \sigma^{-}}{d|t|}}{\frac{d \sigma^{+}}{d|t|}+\frac{d \sigma^{-}}{d|t|}}=p_{1} \cos (\phi) \propto 2 \mathcal{A}_{\mathrm{BH}} \frac{\Re e\left(\mathcal{A}_{\mathrm{DVCS}}\right)}{\left|\mathcal{A}_{\mathrm{DVCS}}\right|^{2}+\left|\mathcal{A}_{\mathrm{BH}}\right|^{2}} \cos (\phi) . \tag{3.69}
\end{equation*}
$$

The measurement of $A_{C}$ is complementary to the measurement of the $|t|$ distribution. The DVCS beam-charge asymmetry has been measured by the H1 648] and HERMES [671, 672] experiments.

The large rapidity acceptance and high precision tracker of the EIC detector together with its very accurate electromagnetic calorimeter and the high luminosity of the machine,
make it an ideal tool for the measurement of both the DVCS cross section differential in $|t|$ and the DVCS+BH cross section asymmetries. Specifically for the BCA, a positron beam would be required.

### 3.9.3 Monte Carlo simulations of DVCS at an EIC

The Monte Carlo generator used for our studies is MILOU 673, which simulates both the DVCS and the BH processes together with their interference term. DVCS is simulated using the framework of GPDs at next-to-leading order (NLO) accuracy, including the NLO evolution of GPDs [625]. The $t$ dependence is introduced as an exponential $d \sigma / d t \propto e^{B\left(Q^{2}\right)|t|}$, where $B\left(Q^{2}\right)$ is either a constant or can have a weak logarithmic dependence on $Q^{2}, B\left(Q^{2}\right) \sim \ln \left(Q^{2}\right)$. In the present simulation, we used the former option, $B\left(Q^{2}\right)=5 \mathrm{GeV}^{-2}$. In addition, the proton dissociation background, ep $\rightarrow e \gamma Y$, has not been included.

The DVCS and BH processes have been simulated in the following kinematic range:

- $Q^{2} \geq 1 \mathrm{GeV}^{2}$;
- $10^{-4}<x_{B}<10^{-1}$;
- $0.01<y<0.85$;
- $0.01<|t|<1 \mathrm{GeV}^{2}$.

The $Q^{2}$ and $x_{B}$ ranges correspond to the phase space achievable with an EIC; the lower $y$ limit is chosen according to the acceptance of the detector; the interval in $|t|$ relates to the acceptance of a forward proton spectrometer. The energy configuration considered for the present study is a $5-20 \mathrm{GeV}$ electron beam colliding with a 250 GeV proton beam.

Figure 3.30 shows the correlation between the scattering angle of the real photon produced in the interaction and its energy for different EIC energy configurations. For the $20 \times 250$ configuration, the photons with an energy greater than $\sim 5 \mathrm{GeV}$ are produced backward at an angle larger than 2.7 rad , corresponding to the rear end-cap calorimeter in the detector. Since for the DVCS process the electron is always scattered backward, this can lead to problems in discriminating the photon and electron clusters and makes it crucial to have an electromagnetic calorimeter with high spatial resolution and a good tracker coverage at backward rapidity to measure the electron track. Indeed, this is extremely important for the $t$ resolution in the case of a measurement performed without a Roman Pots because the four-momentum $t$ must be reconstructed, using momentum conservation, from the transverse momenta of the electron and the photon.

The fraction of BH events has been estimated using an MC sample containing both DVCS and BH processes. The samples have been normalized to the luminosity. The fraction of BH events is calculated as follows:

$$
\begin{equation*}
F_{B H}=\frac{B H_{e v t}}{B H_{e v t}+D V C S_{e v t}} . \tag{3.70}
\end{equation*}
$$

Figure 3.31 shows the fraction of BH events as a function of $y, Q^{2}$, and $|t|$. As expected, DVCS is dominant at low $y$ whereas BH dominates at higher $y$ with its fraction increasing up to $100 \%$ for $y>0.85$.

In the present study, the kinematic domain has been binned logarithmically in $1<Q^{2}<$ $100 \mathrm{GeV}^{2}$ and $10^{-4}<x_{B}<10^{-1}$. Figure 3.32 shows the distribution of the statistics per bin for the $20 \times 250$ configuration (left panel) and $5 \times 50$ configuration (right panel).


Figure 3.30. The angle of the produced real photon in a DVCS event as a function of the photon energy for different EIC energy configurations. Each plot shows also the distribution of the photon and scattered electron energies.


Figure 3.31. The fraction of BH events in the $e p \rightarrow e p \gamma$ sample as a function of $y$ (left), $Q^{2}$ (middle), and $|t|$ (right).



Figure 3.32. The distribution of the DVCS events in a logarithmically binned phase space for the $20 \times 250$ (left) and $5 \times 50$ (right) EIC beam energy configurations.

As an example of the precision that could be achieved at an EIC, figure 3.34 shows the expectations for a measurement of the DVCS ep cross section differential in $|t|, \mathrm{d} \sigma_{e p \rightarrow e p \gamma} / \mathrm{d} t$, for several bins of $x_{B}$ and $Q^{2}$. The estimated luminosity for the $20 \times 250$ configuration is $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. The integrated luminosity of the simulated events is $11.9 \mathrm{fb}^{-1}$, corresponding to approximately one month of running at $20 \times 250$ and assuming $50 \%$ operational efficiency. The $b$ slope parameter with its uncertainty is extracted for each data set via a an exponential fit $\sim e^{-b|t|}$, and its value is reported in figure 3.34 together with uncertainties.

One can see that an excellent measurement (binning over a wide range in $Q^{2}$ and $x_{B}$ ) can already be obtained with a relatively modest beam time, allowing for numerous detailed studies of the reaction mechanism ( $Q^{2}$-scaling behavior, QCD evolution) and extraction of information about the nucleon GPDs and its change with $x_{B}$. The statistical uncertainty for the differential cross section can be, at small $|t|$ values, significantly below $1 \%$, as well as the uncertainty on the extracted slope parameter, $b$. This implies that the measurement is actually limited by systematics. Thus the utilization of a high resolution spectrometer based on the Roman Pots technique becomes important for an EIC. For example, the leading proton spectrometer based on 6 Roman Pots stations equipped with silicon microstrips detectors used at ZEUS for the DVCS $d \sigma / d|t|$ measurement, allowed to measure $P_{t}$ with a resolution of 5 MeV [645] under test beam conditions which corresponded to $\Delta\left(P_{t}^{2}\right)=|\Delta t|=10^{-2} P_{t}$ for a $|t|$ measurement. A new properly designed Roman Pots spectrometer, potentially based on a radiation-hard silicon pixel technology, could reach a geometrical acceptance of about $60 \%$, with a better $P_{t}$ resolution. Since for an EIC systematics are the challenge, it is worth sacrificing the acceptance and therefore increasing the beam time for a more accurate measurement.

Figure 3.35 shows the expectations for a DVCS measurement for large- $|t|$. The data have been simulated for $1<|t|<2 \mathrm{GeV}^{2}$ in several bins of $x_{B}$ and $Q^{2}$. The luminosity of the simulated sample is $151 \mathrm{fb}^{-1}$ corresponding to approximately 52 weeks of data taking in the $20 \times 250$ configuration. One can see that even if the cross section drops drastically for large $|t|$ values, the EIC still allows for good binned measurements, but this requires
years of data taking. (For a relevant discussion, see section (3.6) In this regime, the main detector offers a much better acceptance then Roman Pots and can be used for measuring $|t|$.

A data sample containing DVCS, BH and their interference term has been simulated considering separately an electron beam (luminosity is $44 \mathrm{pb}^{-1}$ ) and a positron beam (luminosity is $47 \mathrm{pb}^{-1}$ ) and used to calculate the beam-charge asymmetry, $A_{C}$. The result is shown in figure 3.33 together with a fit in the form $A_{C}=p_{1} \cos (\phi)$ (3.69), where $p_{1}$ is a free parameter. One can see that a fair accuracy for the BCA can be obtained at an EIC for a modest integrated luminosity.


Figure 3.33. The beam-charge asymmetry $A_{C}$ as a function of the azimuthal angle $\phi$ between the production and scattering planes.


Figure 3.34. The DVCS cross section has been simulated in the range $1.0<Q^{2}<100 \mathrm{GeV}^{2}$, $10^{-4}<x_{B}<0.1$ for the $20 \times 250 \mathrm{GeV}$ energy configuration. The DVCS cross section is simulated in several bins of $x_{B}$ and $Q^{2}$ and is shown for small $|t|$ values.


Figure 3.35. The DVCS cross section has been simulated in the range $1.0<Q^{2}<100 \mathrm{GeV}^{2}$, $10^{-4}<x_{B}<0.1$ for the $20 \times 250 \mathrm{GeV}$ energy configuration. The DVCS cross is section simulated in several bins of $x_{B}$ and $Q^{2}$ and is shown for large $|t|$ values.

### 3.10 DVCS Beam Spin Asymmetries with an EIC

R. Géraud, H. Moutarde, F. Sabatié

### 3.10.1 Deeply Virtual Compton Scattering polarization observables

The photon electroproduction $e p \rightarrow e p \gamma$ can either occur by radiation along one of the electron lines (Bethe-Heitler or BH) or by emission of a real photon by the nucleon (Deeply Virtual Compton Scattering or DVCS). The total cross section as given by 625 reads:

$$
\begin{equation*}
\frac{\mathrm{d} \sigma^{e p \rightarrow e p \gamma}}{\mathrm{~d} x_{B} d y \mathrm{~d} \Delta^{2} \mathrm{~d} \phi \mathrm{~d} \varphi}=\frac{\alpha^{3} x_{B} y}{16 \pi^{2} Q^{2} \sqrt{1+\epsilon^{2}}}\left|\frac{\mathcal{T}}{e^{3}}\right|^{2}, \tag{3.71}
\end{equation*}
$$

where $\Delta$ is the 4 -momentum transfer between the initial and final proton; $Q^{2}$ the virtuality of the exchanged photon; $x_{B}$ the usual Bjorken variable; $\epsilon=2 x_{B} M / Q$ ( $M$ is the proton mass); $y$ is the fraction of the electron energy lost in the nucleon rest frame; $\phi$ is the angle between the leptonic plane $\left(e, e^{\prime}\right)$ and the photonic plane $\left(\gamma^{*}, \gamma\right)$ as shown in figure 3.36 The angle $\varphi$ is defined as the difference between $\phi$ and $\phi_{S}$, the orientation of the target spin in the case of a polarized target, shown also in figure 3.36.


Figure 3.36. Kinematics of the photon leptoproduction in the target rest frame (the Trento notations). The incoming and outgoing leptons define the scattering plane, and the outgoing photon and recoil protons define the hadronic plane. In this reference system, the azimuthal angle between the lepton and recoil proton planes is $\phi$. The angle $\phi_{S}$ defines the orientation of the target spin in the case of a polarized target (it will not be used in the present contribution).

The total amplitude $\mathcal{T}$ is the superposition of the BH and DVCS amplitudes:

$$
\begin{align*}
|\mathcal{T}|^{2} & =\left|\mathcal{T}_{\mathrm{BH}}\right|^{2}+\left|\mathcal{T}_{\mathrm{DVCS}}\right|^{2}+\mathcal{I}, \\
\mathcal{I} & =\mathcal{T}_{\mathrm{DVCS}}^{*} \mathcal{T}_{\mathrm{BH}}+\mathcal{T}_{\mathrm{DVCS}} \mathcal{T}_{\mathrm{BH}}^{*}, \tag{3.72}
\end{align*}
$$

where $\mathcal{T}_{\text {DVCS }}$ and $\mathcal{T}_{\text {BH }}$ are the amplitudes for the DVCS and Bethe-Heitler processes, and $\mathcal{I}$ denotes the interference between these amplitudes. The individual contributions to the total $e p \rightarrow e p \gamma$ cross section can be written as (up to twist- 3 contributions and corrections
in $1 / Q$ ) 625:

$$
\begin{align*}
\left|\mathcal{T}_{\mathrm{BH}}\right|^{2} & =\frac{\Gamma_{\mathrm{BH}}\left(x_{B}, Q^{2}, t\right)}{\mathcal{P}_{1}(\phi) P_{2}(\phi)}\left\{c_{0}^{\mathrm{BH}}+\sum_{n=1}^{2} c_{n}^{\mathrm{BH}} \cos (n \phi)+s_{1}^{\mathrm{BH}} \sin \phi\right\},  \tag{3.73}\\
\left|\mathcal{T}_{\mathrm{DVCS}}\right|^{2} & =\Gamma_{\mathrm{DVCS}}\left(x_{B}, Q^{2}, t\right)\left\{c_{0}^{\mathrm{DVCS}}+\sum_{n=1}^{2}\left[c_{n}^{\mathrm{DVCS}} \cos (n \phi)+s_{n}^{\mathrm{DVCS}} \sin (n \phi)\right]\right\}  \tag{3.74}\\
\mathcal{I} & \left.=\frac{\Gamma_{I}\left(x_{B}, Q^{2}, t\right)}{\mathcal{P}_{1}(\phi) P_{2}(\phi)}\right]\left\{c_{0}^{I}+\sum_{n=1}^{3}\left[c_{n}^{I} \cos (n \phi)+s_{n}^{I} \sin (n \phi)\right]\right\}, \tag{3.75}
\end{align*}
$$

where $\Gamma_{\mathrm{BH}}, \Gamma_{\mathrm{DVCS}}$ and $\Gamma_{I}$ are known kinematical prefactors. $\mathcal{P}_{1}(\phi)$ and $\mathcal{P}_{2}(\phi)$ come from the BH electron propagators and can be written as:

$$
\begin{equation*}
Q^{2} \mathcal{P}_{1}=Q^{2}+2 k \cdot \Delta, \quad Q^{2} \mathcal{P}_{2}=-2 k \cdot \Delta+\Delta^{2}, \tag{3.76}
\end{equation*}
$$

where $k$ is the 4 -momentum of the incoming lepton.
In the case of scattering on unpolarized or longitudinally polarized targets, all $\sin (n \phi)$ coefficients in (3.73(3.75) depend either on the beam helicity $\lambda$ or on the target longitudinal polarization $\Lambda$; they disappear in the unpolarized cross section.

Using a polarized beam, two separate quantities can be extracted: the difference of cross section with opposite beam helicities and the total cross section, which at leading twist can be written respectively as:

$$
\begin{align*}
d \sigma^{\rightarrow}-d \sigma^{\leftarrow} & =2 \cdot \mathcal{T}_{\mathrm{BH}} \cdot \Im m\left(\mathcal{T}_{\mathrm{DVCS}}\right), \\
d \sigma^{\rightarrow}+d \sigma^{\leftarrow} & =\left|T_{\mathrm{BH}}\right|^{2}+2 \cdot \mathcal{T}_{\mathrm{BH}} \cdot \Re e\left(\mathcal{T}_{\mathrm{DVCS}}\right)+\left|T_{\mathrm{DVCS}}\right|^{2}, \tag{3.77}
\end{align*}
$$

where the arrows correspond to the beam helicity. At low $y$, the interference term entering the total cross section is small compared to the DVCS and BH contributions, which contrasts with the case of intermediate or large $y$ where the DVCS contribution is small with respect to the interference, which itself is in general significantly smaller than the BH term. Note that the DVCS contribution to the difference of cross section only appears at higher twist.

From these two natural observables, one can write asymmetries which are experimentally easier to determine than cross sections:

$$
\begin{equation*}
A_{L U}=\frac{d \sigma^{\leftarrow}-d \sigma^{\rightarrow}}{d \sigma^{\leftarrow}+d \sigma^{\rightarrow}}, \tag{3.78}
\end{equation*}
$$

Beam spin asymmetries are mostly sensitive to the GPD $H$ and are complementary to unpolarized cross sections and beam charge asymmetry measurements presented in section 3.9.

### 3.10.2 Monte Carlo

The PROPHET package [674] was used in its Monte Carlo configuration to generate photon electroproduction pseudo-data in the EIC kinematics. We relied on the GoloskokovKroll model for GPDs 605 evaluated at NLO, integrated over the LO hard kernel to obtain Compton Form Factors $\mathcal{H}, \widetilde{\mathcal{H}}, \mathcal{E}$ and $\widetilde{\mathcal{E}}$ which are the complex counterparts of GPDs and directly relate to the DVCS amplitude at the leading order of $\alpha_{s}$ [625]. Note that $\widetilde{\mathcal{E}}$ only enters the unpolarized cross section for DVCS, but was neglected in this evaluation.

The photon electroproduction observables were evaluated using the GV package 675], which in contrast with the usual BMK formalism [625], does not make approximations of the order of $1 / Q$ in the treatment of the interference term. It was checked that the unpolarized cross sections generated by our Monte Carlo give the results simular to those shown in section [3.9, but with more realistic $b$-slopes since they were not taken as a constant but form a part of the Goloskokov-Kroll model.

### 3.10.3 Projected results

The Beam Spin Asymmetry evaluated in a typical $\left(x_{B}, Q^{2}\right)$ bin is shown in figure 3.37 The $\sin \phi$ coefficient turns out 3 to 5 times lower than that at typical lower energy and higher $x_{B}$ kinematics. Therefore, this asks for a rather large integrated luminosity. For the considered $x_{B}$ range (and lower), about three months of EIC at $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ luminosity assuming $50 \%$ operational efficiency is necessary to achieve a 10 to $15 \%$ accuracy on the extracted $\sin \phi$ coefficient, mostly linked to the imaginary part of CFF $\mathcal{H}$. For higher $x_{B}$ and $Q^{2}$ values, much larger integrated luminosities will be necessary to achieve similar statistical accuracy.

Using longitudinal and transverse target asymmetries, one will be able to obtain information on $\widetilde{H}$ and even the elusive $E$, essential for the evaluation of Ji's sum rule. Studies of these observables for the EIC are in progress using the same formalism.


Figure 3.37. Photon electroproduction Beam Spin Asymmetries for the $20 \times 250$ EIC configuration, in the typical kinematic bin: $1.58 \cdot 10^{-3}<x_{B}<2.51 \cdot 10^{-3}, 3.16<Q^{2}<5.61 \mathrm{GeV}^{2}$ for four different $t$-bins as shown on each plot. The Monte Carlo was set up as to generate 90 k events for each $t$-bin and the corresponding integrated luminosity is shown on each plot. Up to about 3 months of beam time with $50 \%$ efficiency is necessary to achieve 10 to $15 \%$ accuracy on the extracted $\sin \phi$ coefficient p0, sensitive to the imaginary part of CFF $\mathcal{H}$.

### 3.11 Hard exclusive photoproduction of Quarkonia

Peter Kroll

Photoproduction of quarkonia (e.g., $J / \Psi$ and $\Upsilon$ ) forms another class of hard exclusive processes which allow one to scrutinize the handbag approach and extract information on generalized parton distributions (GPDs). Neglecting intrinsic heavy quarks in the proton, only the gluonic subprocess $\gamma^{*} g \rightarrow M g$ (accompanied by the gluon GPDs) contributes to the scattering amplitude. A particular feature of quarkonium production is the appearance of the large mass, $m_{Q}$, of the heavy quark which provides a hard scale and allows one to treat photoproduction within a QCD factorization approach. A first leading-order calculation of quarkonium production within the handbag approach has been carried out in 676]. Recently this analysis has been improved by the inclusion of NLO corrections 6677. In these studies, a non-relativistic scenario for the description of the quarkonium state has been adopted in which the quark and antiquark share the meson's momentum equally. Hence, the quarkonium wave function is proportional to $\delta(x-1 / 2)$ and the quarkonium mass is given by $M_{Q} \simeq 2 m_{Q}$. There are other theoretical approaches to the process of interest, e.g., the dipole approach, the leading $\ln (1 / x)$ approximation or the BFKL Pomeron. Due to limitation of space these approaches will not be discussed here.

In the kinematical range of large photon-proton center-of-mass energy, $\sqrt{s} \gg M_{Q}$, and small momentum transfer, $t$, the skewness is given by

$$
\begin{equation*}
\xi=M_{Q}^{2} /(2 s) . \tag{3.79}
\end{equation*}
$$

Neglecting terms of order of $\sqrt{-t} / m_{Q}, t / 4 m^{2}$ and $\xi$, one finds the following expressions for the helicity amplitudes of the quarkonium photoproduction:

$$
\begin{align*}
\mathcal{M}_{\mu+, \mu+} & =\frac{e_{0}}{2} e_{Q} \int_{0}^{1} \frac{d x}{(x+\xi)(x-\xi+i \varepsilon)} \sum_{\lambda} \mathcal{H}_{\mu \lambda, \mu \lambda}\left[H^{g}+\lambda \widetilde{H}^{g}\right] \\
\mathcal{M}_{\mu-, \mu+} & =-e_{0} e_{Q} \frac{\sqrt{-t}}{4 m} \int_{0}^{1} \frac{d x}{(x+\xi)(x-\xi+i \varepsilon)} \sum_{\lambda} \mathcal{H}_{\mu \lambda, \mu \lambda} E^{g} \\
\mathcal{M}_{--,++} & =e_{0} e_{Q} \frac{\sqrt{-t}}{2 m} \int_{0}^{1} \frac{d x}{(x+\xi)(x-\xi+i \varepsilon)} \mathcal{H}_{--,++} H_{T}^{g} . \tag{3.80}
\end{align*}
$$

Other helicity amplitudes are zero except for those related by parity conservation to the above ones. The helicity labels $\mu$ and $\mu^{\prime}$ refer to the initial photon and final meson, respectively; the labels $\lambda$ and $\lambda^{\prime}$ refer to the initial and final gluon, respectively. The explicit helicity labels of $\mathcal{M}$ refer to the proton. In the non-relativistic scenario, the LO subprocess amplitudes read

$$
\begin{equation*}
\mathcal{H}_{\mu^{\prime} \lambda^{\prime}, \mu \lambda}=\frac{8 \pi \alpha_{s}\left(\mu_{R}\right) f_{Q}}{3 m_{Q}} \delta_{\mu^{\prime} \mu} \delta_{\lambda^{\prime} \lambda}, \tag{3.81}
\end{equation*}
$$

where $f_{Q}$ is the decay constant of the quarkonium; $\mu_{R}$ is an appropriate renormalization scale. Thus, at this level of accuracy, only the process amplitudes,

$$
\begin{equation*}
\mathcal{M}_{\mu+, \mu+}=e_{0} e_{Q} \frac{8 \pi \alpha_{s} f_{Q}}{3 m_{Q}}\left\langle H^{g}\right\rangle, \quad \mathcal{M}_{\mu-, \mu+}=-e_{0} e_{Q} \frac{8 \pi \alpha_{s} f_{Q}}{3 m_{Q}} \frac{\sqrt{-t}}{2 m}\left\langle E^{g}\right\rangle \tag{3.82}
\end{equation*}
$$

are non-zero. The terms $\langle F\rangle$ denote the convolutions of the subprocess amplitudes and GPDs. One sees that the unpolarized cross section for quarkonium production at small $t$
is only fed by $H^{g}$, while the asymmetry measured with a transversally polarized target is given by an interference term of $E^{g}$ and $H^{g}$. Other GPDs, like the chiral-odd $H_{T}^{g}$, do not contribute at this level of accuracy.

For the EIC kinematics for which $\xi<0.01$, quarkonium production is a diffractive process, i.e., the amplitudes are dominantly imaginary. Thus, essentially the GPDs are only needed at the cross-over line $x=\xi$, while the small real part may be estimated with the help of analyticity. Many methods for the construction of GPDs, e.g., the double distribution ansatz 678] or the Shuvaev transform [593], lead to GPDs which at $x=\xi$ are proportional to the usual parton distributions. In particular, for the reggeized double distribution ansatz used in [659, 679], one has

$$
\begin{equation*}
H^{g}(\xi, \xi, t)=c_{h}[2 \xi g(2 \xi)](2 \xi)^{-\alpha_{h}^{\prime} t} e^{b_{h} t} \tag{3.83}
\end{equation*}
$$

Assuming that $x g(x)=c x^{-\delta_{h}}$ at low $x$, the constant $c_{h}$ reads (with $b=2$ [678]):

$$
\begin{equation*}
c_{h}=c\left[\left(1-\delta_{h} / 5\right)\left(1-\delta_{h} / 4\right)\left(1-\delta_{h} / 3\right)\right]^{-1} . \tag{3.84}
\end{equation*}
$$

Since $\delta_{h}$ is positive, $c_{h}>c$, which implies that $H^{g}(\xi, \xi, t=0)>2 \xi g(2 \xi)$ (this is termed the skewness effect). In (3.83), a linear gluonic ('Pomeron-like') Regge trajectory is assumed:

$$
\begin{equation*}
\alpha_{h}=1+\delta_{h}+\alpha_{h}^{\prime} t . \tag{3.85}
\end{equation*}
$$

Its slope is taken from the $J / \Psi$ photoproduction data 588 ( $\left.\alpha_{h}^{\prime}=0.15 \mathrm{GeV}^{-2}\right)$, while $\delta_{h}$, the intercept minus 1 , can be fixed from the data on the cross section for electroproduction of $\rho^{0}$ and $\phi$ mesons [680] that behaves as $\sigma \propto s^{2 \delta_{h}}$. The data provide a scale-dependent intercept (see figure 3.38):

$$
\begin{equation*}
\delta_{h}(\mu)=0.1+0.06 \ln \left(\mu^{2} / \mu_{0}^{2}\right), \tag{3.86}
\end{equation*}
$$

where $\mu_{0}=2 \mathrm{GeV}$ and $\mu=Q$ for electroproduction. The scale dependence of $\delta_{h}$ is in agreement with evolution.


Figure 3.38. Left: The intercept of the gluonic trajectory shifted by one unit; the data points are from [680. Right: Various NLO gluon PDFs. The figure is from 681.

The construction of the GPD along the lines described above requires the knowledge of the gluon PDF; in figure 3.38, some recent results for it are shown. For $x$ smaller than
about $10^{-3}$, the errors of most PDFs become very large. The only exception is the CTEQ6 results [82] for which the error stays constant at the level of about $25 \%$ for $x<10^{-2}$. Since the uncertainties of the PDF are conveyed to the GPDs and, hence, to the quarkonium cross section, any prediction of the latter will suffer from huge uncertainties rendering any comparison with experiment meaningless. In order to arrive at reasonable predictions, the following remedial measure has been proposed in 659, 679]: The gluon PDF is expanded as the following series,

$$
\begin{equation*}
x g(x, \mu)=x^{-\delta_{h}(\mu)}(1-x)^{5} \sum_{i=0}^{2} c_{i}(\mu) x^{i / 2} \tag{3.87}
\end{equation*}
$$

and the expansion parameters are fitted to a given PDF for intermediate values of $x$, say, $0.003<x<0.3$, and relevant scales. The power $\delta_{h}$ is fixed at the experimental value (3.86). Applying this prescription to the NLO CTEQ6 PDF [82], one can reproduce the CTEQ6 result for $x<0.003$. Therefore, the CTEQ6 gluon PDF with its errors may be used for numerical predictions. (The same method applied to other current gluon PDFs leads, in most cases and within uncertainties, to the results for cross sections that are in a reasonable agreement with those evaluated using the CTEQ6 PDF [659].)

The calculation of the quarkonium cross section is further complicated by large NLO corrections 677, see figure 3.39. The results shown in figure 3.39 are evaluated from a GPD that is also generated from the NLO CTEQ6 PDF but under the assumption that, at the initial scale, $H^{g}$ is given by the PDF multiplied by an appropriate function of $t$. Evidently, the large NLO corrections necessitate a resummation of higher orders for a reliable prediction of the quarkonium cross section.


Figure 3.39. Left: LO and NLO predictions for the forward $J / \Psi$ photoproduction $v s . \sqrt{s}$ (the figure is from [677). Right: LO prediction using the GPD given in 679, 659, see the text. The green band indicates the uncertainty of the prediction; the data points are from [589, 588].

In order to examine the dependence of the predictions on the GPD used in the calculation, I have repeated the LO order calculation exploiting the GPD proposed in 659, 679] and whose construction is briefly described above. The result, obtained for a scale of $2 m_{Q}$ which is chosen in concord with the construction of the GPD [see (3.86)], overestimates the data but is in agreement with the experimental energy dependence. It however differs strongly from the LO result presented in 677. Similar observations can be made for photoproduction of the $\Upsilon$.

The target asymmetry for quarkonium production may give access to the GPD $E^{g}$, of which not much is known, see the discusion in section 3.4. Indeed,

$$
\begin{equation*}
A_{U T}=-\frac{\sqrt{-t}}{m} \frac{\left|\left\langle E^{g}\right\rangle\right|}{\left|\left\langle H^{g}\right\rangle\right|} \sin \phi, \tag{3.88}
\end{equation*}
$$

where $\phi$ is the relative phase between $\left\langle H^{g}\right\rangle$ and $\left\langle E^{g}\right\rangle$. Since $E^{g}$ is expected to behave similarly to $H^{g}$ at small $\xi$ but with a Regge trajectory $\alpha_{e}=1+\delta_{e}+\alpha_{e}^{\prime} t$, analyticity tells us that the relative phase is approximately given by

$$
\begin{equation*}
\phi(t)=\pi / 2\left(\alpha_{e}(t)-\alpha_{h}(t)\right) . \tag{3.89}
\end{equation*}
$$

In a soft Pomeron scenario, one would have $\alpha_{e}=\alpha_{h}$ and, hence, $A_{U T}=0$. However, the QCD evolution of the GPDs may generate differences in the trajectories and, therefore, $A_{U T}$ may be non-zero. To work this out, one needs a detailed study of the evolution of $E^{g}$, which is lacking at present. There are examples of $\alpha_{e}$ in the literature that lead to tiny asymmetries of the order of $1-2 \%$. In section 3.4, it has been proposed a parameterization of $E^{g}$ with a node at some intermediate value of $x$. In this case one may obtain a larger $A_{U T}$. However, this possibility has not yet been explored in detail.

Summary: Comparing precise data of the cross section for photoproduction of quarkonia with theoretical calculations within the handbag approach may allow for an extraction of $H^{g}$ at the cross-over line and small values of $\xi$ since the real part of the amplitude provides only small corrections to the cross section of the order of $10 \%$. This may lead to a useful constraint on $H^{g}$ and $g(x)$ at low $x$. However, in order to arrive at reliable results for $H^{g}$, the theoretical calculation should include resummed higher orders of perturbative QCD. Also, deviations from the non-relativistic scenario should be investigated and the strength of contributions from intrinsic heavy quarks estimated. Furthermore, a detailed comparison of various gluon GPDs should be made and their errors taken into account. For photoproduction of charmonium production in particular, one should be aware of possible substantial power corrections since the charm quark mass although being large enough to allow for a perturbative treatment of the subprocess, is not large enough to suppress power corrections decisively. On the other hand, for electroproduction of charmonium power corrections are likely to be smaller. In principle the target asymmetry gives an access to $E^{g}$. However, $A_{U T}$ will likely be very small except for the case when $E^{g}$ markedly differs from common parameterizations.

### 3.12 Simulations of non-diffractive exclusive processes at an EIC

## T. Horn

### 3.12.1 Introduction

Exclusive processes in $e p$ scattering at collider energies can be either "diffractive" (no exchange of quantum numbers between the target and the projectile/produced system) or "non-diffractive" (there is an exchange of quantum numbers). By measuring diffractive channels $\left(J / \Psi, \rho^{0}\right.$, or $\phi$ production) at sufficiently high $Q^{2}$, one probes the gluon GPDs and/or the singlet quark GPDs. In particular, $J / \Psi$ production probes the gluon GPD in the nucleon, and its $t$-dependence reveals the transverse spatial distribution of the gluons. Measurements of DVCS and exclusive $\rho^{0}$ production at high $Q^{2}$ provide access to the singlet quark and gluon GPDs.

Non-diffractive channels like $\pi^{+}, \pi^{0}$, or $K^{+}$production are sensitive to the flavor and spin structure of the nucleon at small $x_{B}$, which complements the information obtained from DVCS and meson production experiments in the valence region, e.g., HERMES and 6 GeV and 12 GeV JLab.

For moderate values of $x_{B}$, the proposed electron-ion collider (EIC) could reach $Q^{2}>10$ $\mathrm{GeV}^{2}$, where higher-twist contributions, which complicate the extraction of GPDs from the data, are expected to be small. Indeed, the comparison of different meson channels alone provides model-independent information about the ratio of quark spin and spatial distributions, and a comparison between, for instance, $\pi^{+}$and $K^{+}$production may allow for the studies of $\mathrm{SU}(3)$ symmetry in parton distributions.

### 3.12.2 Rate predictions

Rate predictions were made for several exclusive reaction channels using a new exclusive Monte Carlo generator. Here, we will focus on the $\pi^{+}$and $K^{+}$channels. These are the simplest systems also allowing for comparisons of non-strange and strange distributions similarly to the comparative studies of singlet quarks and gluons with diffractive exclusive channels.

Figure 3.40 shows the simulated cross section for exclusive pion and kaon production in the $5 \times 50 \mathrm{GeV}$ configuration in ep collisions $(\sqrt{s}=31.6 \mathrm{GeV})$ at a luminosity of $10^{34} \mathrm{~cm}^{-2}$ $\mathrm{s}^{-1} \sqrt[3]{3}$, and data taking for 100 days. The simulated data shown here are divided into four $Q^{2}$ bins between 10 and $45 \mathrm{GeV}^{2}$ for a bin in $x_{B}$ between 0.02 and 0.05 . Each $Q^{2}$ bin was divided into nine $-t$ bins. The simulated pion data cover a range in $-t$ up to $1 \mathrm{GeV}^{2}$ with acceptable rates for the assumed run time and luminosity for all $Q^{2}$ bins. The rates in each $Q^{2}$ bin are highest at small values of $-t$ and smallest at high values of $-t$. This makes sense as one of the features of pion production is the dominance of the "pole term" at low $-t$. Furthermore, the pion rate decreases rapidly with higher $Q^{2}$ bins as the cross sections decrease, which is a characteristic behavior of exclusive reactions. However, one should keep in mind that reaching high $Q^{2}$ is needed due to the factorization requirement for studying the transverse spatial structure of sea quarks. The kaon simulated data are presented in the same kinematic bins as the pion data. The kaon cross section is smaller than the pion

[^273]one, although it does not fall off as rapidly with increasing $-t$ for each $Q^{2}$ bin, because the kaon pole is not as dominant as the pion pole. The kaon rates are generally lower than the pion rates, but the effect is most visible in the largest $Q^{2}$ bins. For a fully differential kaon measurement, it is thus essential to have luminosities of at least $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. Given the design parameters of the medium-energy collider, this would correspond to a range in $\sqrt{s}$ between 31 and about 45 GeV .


Figure 3.40. EIC simulations for the exclusive pion and kaon electroproduction cross sections at a electron beam energy of 5 GeV and a proton beam energy of $50 \mathrm{GeV}(\sqrt{s}=31.6 \mathrm{GeV}), 100$ days running, and a luminosity of $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. The points are shown for a bin in $x_{B}$ of 0.02 to 0.05 . The four panels denote bins in $Q^{2}$ (from left to right) of $10-15 \mathrm{GeV}^{2}, 15-20 \mathrm{GeV}^{2}, 25-30 \mathrm{GeV}^{2}$, and $35-40 \mathrm{GeV}^{2}$.

The rate prediction depends to some extent on the cross section models included in the simulation. For pions, a Regge-based cross section model that describes existing data well was used 682. The model dependence of the rate prediction was estimated using a different cross section model based on an empirical parameterization of charged pion data 683. For kaons, the rate estimate was based on the empirical fits to world kaon production data. The resulting uncertainty in the simulated rates was about a factor of two.

### 3.12.3 Kinematic considerations

Measurements in exclusive reactions require, besides knowledge of the beam quantities, information of all particles in the exclusive reaction, i.e., the scattered electron, the scattered meson, and the recoil baryon. Below we will illustrate the kinematic features of exclusive reactions using the $\mathrm{H}\left(e, e^{\prime} \pi^{+}\right) \mathrm{n}$ reaction. However, the kinematic distributions shown are independent of the exclusive channel, and are thus generally applicable to all exclusive reactions (diffractive and non-diffractive).

Figure 3.41 shows the accessible phase space for exclusive reactions in $e p$ collisions for five center of mass energies 4. A cut of $Q^{2}>10 \mathrm{GeV}^{2}$ was applied to focus on the region of interest for transverse spatial structure studies. At a value of $\sqrt{s}=13.8 \mathrm{GeV}$, the meson distribution covers the angular range of about 30-40 degrees at relatively small momentum.

[^274]Up to values of $\sqrt{s}=44.7 \mathrm{GeV}$, which correspond to nearly symmetric collisions, the exclusive meson distribution spreads over a wide angular range, still at a moderate momentum. At even higher values of $\sqrt{s}$, the angular spread is reduced significantly. Indeed, the meson distribution is pushed into a relatively narrow forward cone. Furthermore, the events of interest in this narrow angular range also have very high momentum approaching the beam energy. Exclusive measurements at these large values of $\sqrt{s}$ would thus require the detection of a high energy meson over a very small angular range.


Figure 3.41. The kinematic phase space for light mesons in deep exclusive reactions for different ep collisions. A cut of $Q^{2}>10 \mathrm{GeV}^{2}$ is applied to focus on events needed for studies of transverse spatial distributions. The darker regions in the figures denote regions of the highest intensity. The center of mass energies for the medium energies are $\sqrt{s}=13.8 \mathrm{GeV}, 31.6 \mathrm{GeV}$, and 44.7 GeV , and for the high energies $\sqrt{s}=63.2 \mathrm{GeV}$ and 100 GeV . In this simulation, the direction of the electron beam is toward increasing angles.

The momentum resolution $(d p / p)$ to first order scales linearly with the momentum. The best resolution is thus achieved by keeping the laboratory momenta as low as possible for a given $\sqrt{s}$. This is achieved in symmetric, or nearly symmetric collisions. As illustrated in figures 3.41 and 3.42 such kinematics also offer the advantage that the angular distribution of the outgoing electrons and mesons covers nearly $4 \pi$, providing the best angular resolution.

Figure 3.42 shows the scattered electron distribution in deep exclusive reactions. At modest electron energies (up to about 6 GeV ) electrons predominantly scatter into the central and forward direction. Kinematically these correspond to high- $Q^{2}$ events, which are also the events of interest in studies of the transverse spatial structure of sea quarks. On the other hand, electrons at larger energies (up to the electron beam energy) scatter into the forward-electron direction. These events correspond to low- $Q^{2}$ events, which are of interest in photoproduction or heavy meson measurements.

The meson momentum distribution has a strong $Q^{2}$ dependence with the high momentum region dominated by low- $Q^{2}$ (photoproduction) events. This is illustrated in figure 3.43


Figure 3.42. The kinematic phase space for electrons in exclusive reactions at low and high $Q^{2}$ at a fixed value of $\sqrt{s}=49.0 \mathrm{GeV}$.
with a comparison of photo- and electroproduction at fixed $\sqrt{s}=22 \mathrm{GeV}$ using a cut of $Q^{2}>$ $10 \mathrm{GeV}^{2}$ to select the electroproduced light mesons. The forward scattered photoproduced mesons dominate the low $Q^{2}$ region populating a narrow angle cone with high momentum while the light mesons with $Q^{2}>10 \mathrm{GeV}^{2}$ are centered around central angles at momenta between 2 and 4 GeV . The scattered electron distribution shows the same general features as discussed above. The $t$ distribution of the recoil baryons does not change with selecting the low or high $Q^{2}$ region.


Figure 3.43. A comparison of the kinematic phase space for the scattered meson, electron, and the recoiling baryon in exclusive photo- and meson electroproduction at $\sqrt{s}=21.9 \mathrm{GeV}$. The three upper panels are dominated by photoproduction; the three lower panels focus on light meson events for studies of transverse spatial distributions.

The EIC includes the option of using higher electron energies up to 11 GeV . Figure 3.44 shows a comparison of the meson distribution at fixed values of the ion beam energy for three values of $\sqrt{s}=21.9,31.6,44.7 \mathrm{GeV}$. Here, we will focus on the distribution in the central region, which is indicated by the vertical lines. As mentioned above, the meson distribution is pushed into a narrow angular cone with an increasingly higher momentum as $\sqrt{s}$ increases. Furthermore, the average meson momentum in the central region between $\pm 30 \mathrm{deg}$ increases from $4 \mathrm{GeV} / \mathrm{c}$ to about $8 \mathrm{GeV} / \mathrm{c}$ as the electron beam energy doubles from about 5 to 10 GeV at a fixed ion beam energy. Measurements of exclusive reactions at electron beam energies of about $10 \mathrm{GeV} / \mathrm{c}$ and fixed ion beam energies would thus require the detection of high momentum mesons in the central angle region $\left( \pm 30^{\circ}\right)$.


Figure 3.44. The meson kinematic phase space for higher energies for deep exclusive reactions for different combinations of the beam electron and proton energies. The first value in the labels denotes the electron beam energy. A cut of $Q^{2}>10 \mathrm{GeV}^{2}$ is applied to focus on events needed for studies of transverse spatial distributions.

To access the physics of interest in exclusive reactions and extract information about the GPDs, one needs data binned over a sufficiently large range in $-t$ : a range of at least $0<|t|<1 \mathrm{GeV}^{2}$ is needed. In $e p$ collisions, the main challenge is that the outgoing baryons are scattered at relatively small angles, especially at low $-t$, as the resolution goes roughly as the inverse of the proton beam energy,

$$
\begin{equation*}
\frac{\delta t}{t} \sim \frac{t}{E_{p}} . \tag{3.90}
\end{equation*}
$$

Figure 3.45 illustrates the deep exclusive recoil baryon $-t$ angular resolutions for values of $\sqrt{s}=(13.8,31.6,44.7,63.2,100) \mathrm{GeV}$. The nearly symmetric collisions at lower proton beam energy provide the largest recoil baryon angular distributions of values of at least $1^{\circ}$. For asymmetric collisions, the distribution rapidly decreases to the angular distributions of less than $0.3^{\circ}$. To access the physics of interest, a better $-t$ resolution would thus be achieved with lower-energy and more symmetric kinematics.

### 3.12.4 L/T separation

Beyond studies of transverse spatial structure of sea quarks, non-diffractive processes provide the opportunity for additional studies, for instance, the tests of hard-soft QCD factorization and measurements of the pion form factor. These measurements require isolating the longitudinal part of the electroproduction cross section using the L/T separations. This


Figure 3.45. The kinematic phase space as $-t$ vs. the scattering angle of the recoil baryon in exclusive reactions for five values of $\sqrt{s}$. The first value in the labels denotes the electron beam energy. A cut of $Q^{2}>10 \mathrm{GeV}^{2}$ is applied to focus on events needed for studies of transverse spatial distributions.


Figure 3.46. The virtual photon polarization, $\epsilon$ as a function of $s$ for different combinations of the electron and proton beam energies, at fixed $Q^{2}=10 \mathrm{GeV}^{2}, x_{B}=0.1$, and $-t=0.1 \mathrm{GeV}^{2}$. At high values of $s, \epsilon \rightarrow 1$ complicating the $\mathrm{L} / \mathrm{T}$ separation.
technique requires comparing data taken at two different beam energies with sufficiently large separation of the virtual photon polarization, $\Delta \epsilon$, to control systematic uncertainties. Based on previous $\mathrm{L} / \mathrm{T}$ separations, a minimum acceptable value of $\Delta \epsilon$ is 0.1 .

Figure 3.46 shows the accessible values of $\epsilon$ as a function of $s$ at fixed values of $Q^{2}$, $x_{B}$, and $-t$. The lowest value of $\epsilon$ of about 0.8 is reached at $\sqrt{s}=14.3 \mathrm{GeV}$, increasing to near unity as $s$ increases. Beyond $\sqrt{s}=31.6 \mathrm{GeV}, \epsilon$ is effectively unity making the $\mathrm{L} / \mathrm{T}$ distributions impossible.

### 3.12.5 Summary of basic requirements for exclusive reactions

Studies of exclusive non-diffractive processes provide important information on the transverse spatial distribution of non-perturbative sea quarks. These measurements require high luminosity for fully differential measurements in $x_{B},-t$, and $Q^{2}$ as well as recoil detection for exclusivity. They require a kinematic reach in $t$ of at least up to $1 \mathrm{GeV}^{2}$ with good resolution. Our studies suggest that exclusive processes for values of $x_{B}>0.01$ have better prospects with lower-energy and more symmetric kinematics.

The following list summarizes the basic experimental requirements for studies of the transverse spatial structure of sea quarks through non-diffractive exclusive processes.
Energies

- More symmetric energies favorable in exclusive non-diffractive reactions;
- Lower energies essential for a range in $\epsilon$ for the $\mathrm{L} / \mathrm{T}$ separation.

Kinematic Reach

- Need $Q^{2}>10 \mathrm{GeV}^{2}$ (pointlike configurations);
$-x_{B}$ range between 0.001 and 0.1 overlapping with HERA and JLab 12 GeV ;
$-s$ range between 200 and $1000 \mathrm{GeV}^{2}$.
Luminosity
- Exclusive non-diffractive processes require high luminosity for low rates for fully differential measurements; - Kaons push luminosity to $>10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$.
Detection
- Need recoil detection for exclusivity;
- Range in $-t$ and resolution.


# 3.13 Partonic transverse spin in deep-inelastic exclusive experiments 

Gary R. Goldstein, Simonetta Liuti

### 3.13.1 Introduction

In this contribution, we suggest a class of deeply virtual exclusive reactions, namely pseudoscalar meson electroproduction, as a means to access chiral-odd distributions. These are described by a set of four chiral-odd GPDs which enter the matrix elements for the various terms of the cross section. We conducted an analysis using a parameterization of the GPDs that is inspired by a physically motivated picture of the nucleon as a quark-diquark system with a Regge behavior. In the chiral-even sector a quantitative parameterization can be obtained from a global fit to PDFs, nucleon form factors, and DVCS data where the masses, couplings and Regge power behavior that set the scale for the dependence on the kinematic variables, $X, \zeta, t, Q^{2}$, are determined via a recursive procedure [684].

The extension of this parameterization scheme to the chiral-odd GPDs is critical for the phenomenology of deeply virtual meson electroproduction, which was begun particularly for the $\pi^{0}$ in [685]. In the diquark spectator model, chiral-even helicity amplitudes are simply related to their chiral-odd counterparts via parity transformations. For the $d$-quark case it is only the axial diquark relations that are involved, while the $u$-quark involves the scalar contribution, as well. We thereby obtain the full set of four chiral-odd GPDs, each being linearly related to helicity amplitudes. This allows us to predict the behavior of pseudoscalar electroproduction 686].

It has now become particularly pressing to study the heavy quark components of the nucleon because of the advent of the LHC. For the types of precision measurements in the unprecedented multi- TeV CM energy regimes envisaged at the LHC it will be necessary to provide accurately determined QCD inputs. The analyses in 129 have shown how the inclusion of non perturbative charm quarks could modify the outcome of global PDF analyses. However, the situation is not clear-cut. We therefore extended our analysis to strange and charm pseudoscalar meson production [687]. We proposed that in order to refine analyses such as the one in [129], new observables need to be identified from deeply virtual meson production and spin correlation measurements. We presented preliminary results involving the following electroproduction exclusive processes: (1) $\gamma^{*} p \rightarrow J / \psi p^{\prime}$; (2) $\gamma^{*} p \rightarrow D \bar{D} p^{\prime} ;(3) \gamma^{*} p \rightarrow \bar{D} \Lambda_{c}$; (4) $\gamma^{*} p \rightarrow \eta_{C} p^{\prime}$. These processes necessitate: i) high luminosity because they are exclusive; ii) high enough $Q^{2}$ to produce the various charmed mesons, and iii) a wide kinematical range in Bjorken $x$.

Finally, a few questions have emerged concerning on one side the applicability of dispersion relations to deeply virtual exclusive processes [688], and on the other, the commonly assumed partonic picture of the ERBL region [689]. Newer deeply virtual exclusive cross section and asymmetry measurements in extended kinematical regimes will provide essential tests of the theory.

### 3.13.2 Transverse spin from pseudoscalar meson production

The basic definition of the quark-nucleon GPDs is through off-forward matrix elements of quark field correlators. Contracting with the Dirac matrices, $\gamma^{\mu}$ or $\gamma^{\mu} \gamma^{5}\left(\sigma^{\mu \nu} \gamma^{5}\right)$, and integrating over the internal quark momenta gives rise to the four chiral-even GPDs, $H, E$
or $\widetilde{H}, \widetilde{E}$, and four chiral-even GPDs, $H_{T}, E_{T}, \widetilde{H}_{T}, \widetilde{E}_{T}$ [575]. The crucial connection of the eight GPDs to spin dependent observables in DVCS and DVMP is through the helicity decomposition 575. For example,

$$
\begin{gather*}
A_{++,++}(X, \xi, t)=\frac{\sqrt{1-\xi^{2}}}{2}\left(H^{q}+\tilde{H}^{q}-\frac{\xi^{2}}{1-\xi^{2}}\left(E^{q}+\tilde{E}^{q}\right)\right),  \tag{3.91}\\
A_{++,--}(X, \xi, t)=\sqrt{1-\xi^{2}}\left(H_{T}^{q}+\frac{t_{0}-t}{4 M^{2}} \tilde{H}_{T}^{q}-\frac{\xi}{1-\xi^{2}}\left(\xi E_{T}^{q}+\tilde{E}_{T}^{q}\right)\right) . \tag{3.92}
\end{gather*}
$$

We have constructed a robust model for the GPDs, extending previous work [690 that is based on the parameterization of diquark spectators and Regge behavior at small $X$. The GPD model parameters are constrained by their relations to PDFs (at $\zeta=0, t=0$ ) and to nucleon form factors $F_{1}(t), F_{2}(t), g_{A}(t)$, and $g_{P}(t)$ through the first $x$ moments. For the chiral-odd GPDs, there are fewer constraints. In particular, $H_{T}(X, 0,0)=h_{1}(X)$ can be fit using the loose constraints in [250] since the first moment of $H_{T}(X, \xi, t)$ is the "tensor form factor", called $g_{T}(t)$. It is conjectured that the first moment of $2 \tilde{H}_{T}^{q}(X, 0,0)+E_{T}^{q}(X, 0,0)$ is a "transverse anomalous moment", $\kappa_{T}^{q}$, defined in [497].

With our ansatz, many observables can be determined in parallel with the corresponding Regge predictions. Since the initial work [685], we have undertaken a more extensive parameterization and presented several new predictions [684. In figure 3.47, we show an example corresponding to the transversely polarized proton target.


Figure 3.47. Left: Transverse spin asymmetry, $A_{U T}$, vs. $-t$ at $Q^{2}=2.3 \mathrm{GeV}^{2}$ and $x_{B}=0.36$ for different values of the tensor charge, $\delta u$, with fixed $\delta d=-0.62$. Right: Comparison of $\pi^{0}$ and $\eta_{c}$ cross sections. The range between the two lines gives an estimate of where the cross sections for the other processes will lie.

The measured cross section for $\pi^{0}$ is sizable and has large transverse $\gamma^{*}$ contributions. This indicates that the main contributions should come from chiral-odd GPDs, for which the $t$-channel decomposition is richer. In particular, because these GPDs arise from the Dirac matrices $\sigma^{\mu \nu}$, there are two series of $J^{P C}$ values for each GPD 691] corresponding to spacespace or time-space combinations $1^{--}$and $1^{+-}$. These series occur for three of the four chiral-odd GPDs, with exception of $\widetilde{E}_{T}$. We are thus led to the conclusion that chiral-odd GPDs will dominate the neutral pseudoscalar leptoproduction cross sections. This result
has interesting consequences. First, in a factorized handbag picture, these GPDs will couple to the hard part, the $\gamma^{*}+$ quark $\rightarrow \pi^{0}+$ quark, provided that $\pi^{0}$ couples through $\gamma^{5}$, which is naively twist-three, rather than the twist-two coupling $\gamma^{+} \gamma^{5}$. Second, the vector $1^{--}$and axial-vector $1^{+-}$in the $t$-channel, viewed as particles ( $\rho^{0}, \omega$ and $b_{1}^{0}, \mathrm{~h}$ ), couple primarily to the transverse virtual photon. For Reggeons, the $1^{--}$does not couple at all to the longitudinal photon, while the axial-vector $1^{+-}$does so through helicity flip 692. Guided by these observations 685], we assume that the hard part depends on whether the exchange quantum numbers are in the vector or axial-vector series, thereby introducing orbital angular momentum into the model. We use $Q^{2}$ dependent electromagnetic "transition" form factors for vector or axial-vector quantum numbers going to a pion. We calculate these using pQCD for $q+\bar{q}+\gamma^{*}\left(Q^{2}\right) \rightarrow q+\bar{q}$ and a standard $z$-dependent pion wave function, convoluted in the impact parameter representation that allows orbital excitations to be easily implemented.

With our model for the chiral-odd spin-dependent GPDs and these transition form factors, we can obtain the full range of cross sections and asymmetries in kinematic regimes that coincide with ongoing JLab experiments. (A similar emphasis on chiral-odd contributions for $\pi$ electroproduction has recently been proposed 693], although the details of that model are quite different from ours.) We are able to predict the important transverse photon contributions to the observables [685]. In figure 3.47 (left), we show one striking example of the predictions that depend on the values of the tensor charges, thereby providing a means to narrow down those important quantities. This program has been presented 684 and further details will soon appear, as the refinements of the chiral-odd parameterization are completed [686]. In figure 3.47 (right), we show the cross section, $\sigma_{T}+\epsilon \sigma_{L}$, for charmed meson production and compare it to the one for $\pi^{0}$ production 687.

In summary, through the use of physically motivated models and the new horizons provided by the EIC, a far reaching interpretation of the separate spin-dependent GPDs and thereby, a picture of the transverse structure of the nucleons will emerge. The connection of chiral-odd GPDs to the transversity structure of the nucleon is of great interest as a manifestation of quark and gluon orbital angular momentum.

### 3.14 Ways to access transversity GPDs at the EIC

B. Pire, L. Szymanowski, S. Wallon

### 3.14.1 Introduction

Transversity quark distributions in the nucleon remain among the most unknown leading twist hadronic observables. This is mostly due to their chiral-odd character which enforces their decoupling in most hard amplitudes. Generalized parton distributions (GPDs) offer a new way to access the transversity dependent quark content of the nucleon. The factorization properties of exclusive amplitudes allow in principle to extract the four chiral-odd transversity GPDs [694], $H_{T}, E_{T}, \tilde{H}_{T}, \tilde{E}_{T}$. However, one-photon or one-meson electroproduction leading twist amplitudes are insensitive to them [695, 696]. The strategy which we followed in [697, 698] is to study the leading twist contribution to exclusive processes where more mesons are present in the final state. Note that, contrarily to transversity PDFs, transversity GPDs enter the formulae for exclusive cross sections even when considering unpolarized proton target, provided one selects the polarization state of an outgoing meson.

### 3.14.2 Diffractive photoproduction of two $\rho$ mesons

We consider 697, 698], in analogy with the virtual photon exchange occurring in the deep inelastic electroproduction of a meson, the subprocess:

$$
\begin{equation*}
\mathbb{P}\left(q_{P}\right)+p\left(p_{2}\right) \rightarrow \rho_{T}\left(p_{\rho}\right)+N^{\prime}\left(p_{2^{\prime}}\right) \tag{3.93}
\end{equation*}
$$

of almost forward scattering of a virtual Pomeron (the hard scale is the virtuality $-q_{P}^{2}$ of this Pomeron) on a nucleon. This subprocess is at work in the process

$$
\begin{equation*}
\gamma_{L / T}^{(*)}(q)+p\left(p_{2}\right) \rightarrow \rho_{L, T}^{0}\left(q_{\rho}\right)+\rho_{T}\left(p_{\rho}\right)+N^{\prime}\left(p_{2^{\prime}}\right) \tag{3.94}
\end{equation*}
$$

where a real or virtual photon scatters on a proton $p$, which leads via a two-gluon exchange to the production of two vector mesons separated by a large rapidity gap and the scattered nucleon $N^{\prime}$, as shown on figure 3.48. The final state may be either $\rho^{0} \rho^{0} p$ or $\rho^{0} \rho^{+} n$. In both cases, the two-gluon exchange with the nucleon line is forbidden by charge conjugation or charge conservation and the process is thus sensitive only to quark GPDs. We consider the kinematical region where the rapidity gap between $\rho\left(p_{\rho}\right)$ and $N^{\prime}$ is much smaller than the one between $\rho\left(q_{\rho}\right)$ and $\rho\left(p_{\rho}\right)$, i.e., the energy of the $\left(\rho\left(p_{\rho}\right)+N^{\prime}\right)$ system is smaller than that of the $(\rho+\rho)$ system but is still large enough to justify our approach (in particular, it is much larger than baryonic resonance masses). Since quasi-real transverse photons are more abundant in electron-ion collisions and charged pions are most easily detected, one may specialize to the reaction:

$$
\begin{equation*}
\gamma_{T}(q)+p\left(p_{2}\right) \rightarrow \rho_{L, T}^{0}\left(q_{\rho}\right)+\rho_{T}^{0}\left(p_{\rho}\right)+p\left(p_{2^{\prime}}\right) \tag{3.95}
\end{equation*}
$$

where the initial quasi-real photon is treated as if it were real.
In this kinematical regime, the amplitude for this process is calculable consistently within the collinear factorization method, as an integral (over the longitudinal momentum fractions of the quarks) of the product of two amplitudes: the first one (the impact factor) describes the transition $\gamma^{(*)} \rightarrow \rho_{L, T}^{0}$ via a two-gluon exchange and the second one describes the subprocess $\mathbb{P}+p \rightarrow \rho_{T}^{0}+p$. The fact that the latter process is closely related to


Figure 3.48. Factorization of the process $\gamma_{T}(q)+p\left(p_{2}\right) \rightarrow \rho_{L, T}^{0}\left(q_{\rho}\right)+\rho_{T}^{+}\left(p_{\rho}\right)+n\left(p_{2^{\prime}}\right)$ in the asymmetric kinematics discussed in the text. $\mathbb{P}$ is the hard Pomeron modeled by a two-gluon exchange.
the electroproduction process $\gamma^{*} p \rightarrow \rho^{0} p$ allows us to separate its long distance dynamics expressed through the GPDs from a perturbatively calculable coefficient function. The skewness parameter $\xi$ is related in the usual way $\left(\xi \approx x_{B} /\left(2-x_{B}\right)\right)$ to the Bjorken variable defined by the Pomeron momentum $x_{B}=-q_{P}^{2} /\left(2 q_{P} \cdot p_{2}\right)$. The choice of a transversely polarized vector meson $\rho_{T}^{0}$ involves a chiral-odd distribution amplitude, which in turn selects the chiral-odd GPDs.

The resulting scattering amplitude $\mathcal{M} \gamma^{*} p \rightarrow \rho_{L}^{0} \rho_{T}^{0} p$ then receives contributions from the four chiral-odd GPDs $H_{T}, \tilde{H}_{T}, E_{T}$ and $\tilde{E}_{T}$, but only the first one does not vanish kinematically in the forward direction. Thus, assuming that the Mandelstam variable $-t=$ $-\left(p_{2}-p_{2^{\prime}}\right)^{2}$ is sufficiently small, the transversity GPD $H_{T}$ contribution dominates the amplitude of process (3.95) which reads :

$$
\begin{align*}
& \mathcal{M}^{\gamma p \rightarrow \rho_{L}^{0} \rho_{T}^{0} p}=\sin \theta 16 \pi^{2} s \alpha_{s} f_{\rho}^{T} \xi \sqrt{\frac{1-\xi}{1+\xi}} \frac{C_{F}}{N\left(p_{T}^{2}\right)^{2}} \\
& \times \int_{0}^{1} \frac{d u \phi_{\perp}(u)}{u^{2} \bar{u}^{2}} J^{\gamma \rightarrow \rho_{L}^{0}}\left(u p_{T}, \bar{u} p_{T}\right) \frac{H_{T}^{u d}(\xi(2 u-1), \xi, t)}{\sqrt{2}}, \tag{3.96}
\end{align*}
$$

where $H_{T}^{u d}=H_{T}^{u}-H_{T}^{d} ; \phi_{\perp}(u)$ is the distribution amplitude ( DA ) of the $\rho_{T}$ meson; $\theta$ is the angle between the transverse polarization vector of the target $\vec{n}$ and the polarization vector $\vec{\epsilon}_{T}$ of the produced $\rho_{T}^{0}$ meson; $\vec{\varepsilon}$ is the polarization vector of the initial photon. The impact factor reads

$$
\begin{equation*}
J^{\gamma \rightarrow \rho_{L}}\left(k_{T 1}, k_{T 2}=p_{T}-k_{T 1}\right)=-\frac{e \alpha_{s} \pi f_{\rho}^{0}}{\sqrt{2} N} \int_{0}^{1} d z(2 z-1) \phi_{\|}(z)\left(\vec{\varepsilon} \cdot \vec{Q}_{P}\right) \tag{3.97}
\end{equation*}
$$

with

$$
\begin{gathered}
\vec{Q}_{P}\left(k_{T 1}, k_{T 2}=p_{T}-k_{T 1}\right)=\frac{z \vec{p}_{T}}{z^{2} p_{T}^{2}+Q^{2} z \bar{z}+m_{q}^{2}}-\frac{\bar{z} \vec{p}_{T}}{\bar{z}^{2} p_{T}^{2}+Q^{2} z \bar{z}+m_{q}^{2}} \\
+\frac{\vec{k}_{T 1}-z \vec{p}_{T}}{\left(k_{T 1}-z p_{T}\right)^{2}+Q^{2} z \bar{z}+m_{q}^{2}}-\frac{\vec{k}_{T 1}-\bar{z} \vec{p}_{T}}{\left(k_{T 1}-\bar{z} p_{T}\right)^{2}+Q^{2} z \bar{z}+m_{q}^{2}}
\end{gathered}
$$

The scattering amplitude (3.96) receives a contribution only from the ERBL region.

### 3.14.3 Cross section estimates

To obtain an estimate of the differential cross section of this process, we need a model for the transversity GPD $H_{T}^{q}(x, \xi, t)(q=u, d)$. We proposed a simple meson-pole approach starting with the effective interaction Lagrangian,

$$
\begin{equation*}
\mathcal{L}_{\mathcal{A N N}}=\frac{g_{A N N}}{2 M} \bar{N} \sigma_{\mu \nu} \gamma_{5} \partial^{\nu} A^{\mu} N \tag{3.98}
\end{equation*}
$$

in which $g_{A N N}$ is the coupling constant determining the strength of the interaction of the axial meson $A$ with the nucleon $N$. This yields

$$
\begin{equation*}
H_{T}^{a}(x, \xi)=\frac{g_{A N N} f_{A}^{a \perp}\left(\Delta \cdot S_{T}\right)^{2}}{2 M_{N} m_{A}^{2}} \frac{\phi_{\perp}\left(\frac{x+\xi}{2 \xi}\right)}{2 \xi}, \tag{3.99}
\end{equation*}
$$

where $\Delta$ is the transverse part of the momentum transfer vector $r ; f_{A}^{a \perp}$ is related to the $A$ meson decay constant. Identifying the scalar product $\left(\Delta \cdot S_{T}\right)^{2}$ with the average of the intrinsic transverse momentum of the quarks, $\left(\Delta \cdot S_{T}\right)^{2} \rightarrow 1 / 2\left\langle k_{\perp}^{2}\right\rangle$, and the axial meson $A$ with the $b_{1}$ meson, $A=b_{1}(1235)$, we obtain our final expression for $H_{T}^{u d}$ :

$$
\begin{equation*}
H_{T}^{u d}(x, \xi, 0)=\frac{g_{b_{1} N N} f_{b_{1}}^{T}\left\langle k_{\perp}^{2}\right\rangle}{2 \sqrt{2} M_{N} m_{b_{1}}^{2}} \frac{\phi_{\perp}^{b_{1}}\left(\frac{x+\xi}{2 \xi}\right)}{2 \xi}, \tag{3.100}
\end{equation*}
$$

where $f_{b_{1}}^{T}=\sqrt{2} f_{a_{1}} / m_{b_{1}}$ with $f_{a_{1}}=(0.19 \pm 0.03) \mathrm{GeV}^{2} ; g_{b_{1} N N}=5 /(3 \sqrt{2}) g_{a_{1} N N}$ with $g_{a_{1} N N}=7.49 \pm 1.0 ;\left\langle k_{\perp}^{2}\right\rangle=(0.58-1.0) \mathrm{GeV}^{2}$. The $t$ dependence of the chiral-odd GPDs may be parameterized in the following simple way:

$$
\begin{equation*}
H_{T}^{q}(x, \xi, t)=H_{T}^{q}(x, \xi, t=0) \times \frac{C^{2}}{(t-C)^{2}} \tag{3.101}
\end{equation*}
$$

with the standard dipole form factor with $C=0.71 \mathrm{GeV}^{2}$.
In figure 3.49, we show our model estimates for the differential cross sections of photoproduction of two vector mesons (3.94), $\rho^{0}$ and transversely polarized $\rho^{+}$, with the unpolarized beam and target. Note that these cross sections depend on the $\gamma$-nucleon energy only through the variable $\xi$. The cross sections for the processes with two neutral $\rho^{0}$ mesons in the final state are two times smaller than those with $\rho^{0} \rho^{+}$.

### 3.14.4 Photoproduction at lower photon energies

Diffractive physics requires high photon energies. If low energy photon tagging may be performed at the EIC, a QCD study based solely on the collinear factorization (i.e., without any Pomeron exchange) approach may be followed, opening other interesting channels. In 699, 700, we considered the process:

$$
\begin{equation*}
\gamma(q)+p\left(p_{1}, \lambda\right) \rightarrow \pi^{+}\left(p_{\pi}\right)+\rho_{T}^{0}\left(p_{\rho}\right)+n\left(p_{2}, \lambda^{\prime}\right) \tag{3.102}
\end{equation*}
$$

on a polarized or unpolarized proton target, in the kinematical regime of large invariant mass $M_{\pi \rho}$ of the final meson pair (the hard factorization scale is now this invariant mass) and small momentum transfer $t=\left(p_{1}-p_{2}\right)^{2}$ between the initial and the final nucleons. Roughly speaking, this kinematics means a moderate-to-large, and approximately opposite, transverse momentum of each meson. The cross sections obtained are sizeable at values of


Figure 3.49. The differential cross section for the photoproduction of $\rho_{T}^{0}$ and $\rho_{T}^{+}$(left panel) and $\rho_{L}^{0}$ and $\rho_{T}^{+}$(right panel) as a function of $\xi$ for $p_{T}^{2}=2,4$, and $6 \mathrm{GeV}^{2}$. The cross sections for the processes with two neutral $\rho^{0}$ mesons in the final state are two times smaller than those with $\rho^{0} \rho^{+}$.
$s_{\gamma N}$ of the order $10-20 \mathrm{GeV}^{2}$ but decrease quickly with the photon energies. This regime is more in the range of the JLab 12 program than of EIC.

In conclusion, we stress that this approach only assumes leading twist factorization of non-perturbative quantities, such as meson DAs and chiral-odd GPDs.
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## Chapter 4

## Input from lattice QCD

Chapter editors:
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### 4.1 Introduction

Philipp Hägler, Bernhard Musch, Andreas Schäfer

The focus of research at an EIC is a precise and comprehensive understanding of the quark-gluon structure and dynamics of hadrons and nuclei within the scope of traditional QCD, as well as beyond it, e.g., beyond the formalism based on collinear parton distributions. This requires the combination of input from many different fields, including lattice QCD (LQCD). In this chapter, the status of LQCD as well as the prospects for the next decade are sketched. The main tasks of LQCD is to increase precision and to extend the scope of LQCD calculations. [Both depends also significantly on progress in the understanding of perturbative QCD (pQCD).] Although working out solutions for all technical details is a formidable task, recent developments suggest that LQCD should have settled most of the open theory issues by the time the EIC starts operating.

LQCD results are by now routinely used as input for phenomenology if direct experimental information is not available. This trend will intensify when in the future ever more subtle aspects are investigated. Therefore, the EIC and a dedicated effort in LQCD have to form a strong union. If direct comparison with experiment has proven certain types of LQCD calculations to be reliable, LQCD can provide easily information which is hard to obtain experimentally, for example on moments of PDFs and GPDs and the flavour decomposition of structure functions. In this context it is, unfortunately, quite often not sufficiently appreciated that most quantities of interest calculated on the lattice can only be linked to experiment by highly non-trivial input from pQCD. Thus all three elements, experiment, LQCD and pQCD have to be combined to reach optimal results.

The two main sources of difficulty are:

- The basis of LQCD is the observation that the analytic continuation to imaginary times $x^{0} \rightarrow \mathrm{i} x^{4}$ relates quantum field theory to statistics/thermodynamics. The latter allows for a purely numerical treatment by means of Monte Carlo techniques. This analytic continuation is only simple for time-independent quantities. The quantities of this type usually studied are matrix elements of local operators (which can be evaluated at $x^{0}=0=x^{4}$ ).

$$
\begin{equation*}
\left\langle h^{\prime}\left(p^{\prime}\right)\right| \mathcal{O}(x=0)|h(p)\rangle . \tag{4.1}
\end{equation*}
$$

Here $h, h^{\prime}$ can be any hadronic state, including the QCD vacuum. One typically needs the continuum operator product expansion (OPE) to link such quantities to observables.

- Most QCD quantities of interest are scheme and scale dependent. Only in leading order (LO) this dependence can be neglected, but LO calculations are in most cases insufficient for a high precision machine like the EIC. Thus LQCD results for matrix elements of the type Eq. (4.1) have to be matched to a specific pQCD setting, typically the $\overline{M S}$ scheme at a certain scale $\mu$. This requires also a matching of renormalization effects, which are quite different in the continuum and on the lattice due to the loss of continuum symmetries (as discussed below). The lattice discretization leads to different Feynman rules, in particular the appearance of tadpole diagrams. Another concrete, simple example is the modification of the fermion propagator on the lattice,


Figure 4.1. Sketch of the different types of lattice observables. For nearly all quantities of interest for an EIC, a combination of pQCD and LQCD is needed to make contact to experiment.
which typically might read (depending on the specific lattice action)

$$
\begin{equation*}
D_{\text {Lattice }}(p)=\frac{m-\mathrm{i} a^{-1} \sum_{\mu} \gamma_{\mu} \sin \left(p_{\mu} a\right)}{m^{2}+a^{-2} \sum_{\mu} \sin ^{2}\left(p_{\mu} a\right)} \tag{4.2}
\end{equation*}
$$

Thus, renormalization factors on the lattice and in the continuum differ by finite amounts, typically of the order of a few up to 30 percent. If one aims at an overall precision of order percent, the matching of the renormalization factors between nonperturbative (i.e. all order) lattice calculations and fixed order continuum calculations has to be achieved with high precision. To achieve this for all quantities of interest is clearly one of the major challenges for theory, both LQCD and pQCD, in the next decade.

The points just discussed apply to 'indirect observables', as illustrated in the right column of Fig. 4.1. There do also exist some observables which can be compared directly, without the need for renormalization, especially hadron masses. However, these are well known experimentally, while the aim of LQCD is clearly to provide information on hitherto unknown correlators. The observables of interest at the EIC, require nearly always nonperturbative renormalization in the corresponding lattice studies.

The calculation of matrix elements like (4.1) proceeds as follows:

1. One generates a number of ensembles of gauge field configurations with the correct statistical weights. The parameters for these ensembles are chosen such that one has best control (for given computer resources) of the combined limit: lattice spacing $a \rightarrow 0$; physical lattice size $L \gg 1 / \Lambda_{Q C D}$; quark masses $m_{q} \rightarrow m_{q}($ physical $)$; large number of independent field configurations, typically $N \gg 100$.
2. One generates hadronic states using products of quark fields with the correct quantum numbers (sources), e.g., one can use for a proton $\left(C=i \gamma^{2} \gamma^{4}\right.$ is the charge conjugation matrix, $i, j, k$ run over the three color states):

$$
\begin{equation*}
\hat{B}_{\alpha}(t, \vec{p})=\sum_{\vec{x}} e^{\mathrm{i} \vec{p} \cdot \vec{x}} \epsilon_{i j k} \hat{u}_{\alpha}^{i}(x) \hat{u}_{\beta}^{j}(x)\left(C^{-1} \gamma_{5}\right)_{\beta \gamma} \hat{d}_{\gamma}^{k}(x) \tag{4.3}
\end{equation*}
$$

Propagation in Euclidean time generates real exponentials rather than phases. Consequently, when expanding into a series in the correct physical multi-particle hadronic states, propagation in Euclidean time filters out the lowest mass state for large enough times,

$$
\begin{align*}
\hat{B}(0, \vec{p})|0\rangle & =c_{0}|N\rangle+c_{1}\left|N^{\prime}\right\rangle+c_{2}|N \pi\rangle+\ldots \\
\hat{B}(t, \vec{p})|0\rangle & =c_{0} e^{-E_{N} t}|N\rangle+c_{1} e^{-E_{N^{\prime}} t}\left|N^{\prime}\right\rangle+c_{2} e^{-E_{N \pi} t}|N \pi\rangle+\ldots \\
& \sim c_{0} e^{-E_{N^{t} t}}|N\rangle \tag{4.4}
\end{align*}
$$

To improve signals and to investigate higher lying states one uses a set of sources and calculates a full correlation matrix.
3. One constructs ratios for quantities of interest in which the exponential factors cancel, e.g.,

$$
\begin{equation*}
\frac{\tilde{\Gamma}_{\alpha \beta}\left\langle B_{\beta}(t, \vec{p}) \mathcal{O} \bar{B}_{\alpha}(0, \vec{p})\right\rangle}{\Gamma_{\alpha \beta}\left\langle B_{\beta}(t, \vec{p}) \bar{B}_{\alpha}(0, \vec{p})\right\rangle} . \tag{4.5}
\end{equation*}
$$

4. Finally, one determines the relevant renormalization factors for the operator $\mathcal{O}$ nonperturbatively on the lattice and relates the lattice results to a specific pQCD scheme.

One has to appreciate that the efficient combination of experimental and LQCD results requires a good and efficient parametrization for the quantities of interest. If there exists e.g. an efficient parametrization of a specific GPD etc. in terms of just a few parameters, each result will constrain the acceptable parameter range . Thus also high quality model building is necessary.

Over the years it became clear that it is very non-trivial to derive realistic estimates, in particular of the systematic uncertainties, from the highly correlated quantities extracted from Lattice Monte Carlo data. The ultimate test revealing potentially underestimated systematic uncertainties is the comparison of certain benchmark observables with experimental measurements, in this case, EIC data. The next best option is to compare results obtained with substantially different lattice formulations. In principle, each analysis should be repeated at least once with a different action. The latter is typically done in such a way that different collaborations specialise on one specific action each.

The most critical extrapolation is the continuum limit $a \rightarrow 0$. Lattice actions violate basic symmetries of QCD (isotropy and homogeneity of space-time, chiral symmetry, isospin symmetry in the case of twisted-mass fermions ...) for finite lattice spacing. Thus the $a \rightarrow 0$ limit, which restores all symmetries, could be non-trivial. Unfortunately, $a$ can only be varied in very limited ranges because the needed CPU time is always proportional to a large power of $1 / a$. Therefore, a variety of improved lattice actions was proposed in which lattice artifacts are not proportional to $a$ but e.g. $a^{2}$. Many variants exist, all of which are well motivated in one way or the other. Substantial effort is invested to further improve such actions, and it would be very surprising if by the time an EIC starts operating also the systematic uncertainties due to the multiple extrapolation $a \rightarrow 0, L \rightarrow \infty$, $m_{q} \rightarrow m_{q}$ (physical). were not much better under control.
The purely statistical uncertainty will for sure become much smaller due to increased computer power. While the most powerful present day computers are of the Petaflop class, various initiatives aim already at Exaflop computing. In the next sections we will discuss in detail some of the physics quantities calculated on the lattice, which are especially important for the EIC.

### 4.2 Generalized form factors

Most correlators relevant for hadron structure which were determined on the lattice are related to Generalized Parton Distributions (GPDs) or Distribution Amplitudes (DAs). For GPDs the hadronic states in Eq. (4.1) are equal, $h=h^{\prime}$ but the momenta are usually different $\left(p \neq p^{\prime}\right)$. For the best known GPDs $H_{q}$ and $E_{q}$,

$$
\begin{align*}
& \left.\int \frac{d z^{-}}{2 \pi} e^{i x \bar{P}^{+} z^{-}}\left\langle P_{2}\right| \bar{q}\left(-\frac{1}{2} z\right) \gamma^{+} q\left(\frac{1}{2} z\right)\left|P_{1}\right\rangle\right|_{z^{+}=0, z_{\perp}=0} \\
= & \frac{1}{P^{+}}\left[H_{q}(x, \xi, t) \bar{N}\left(P_{2}\right) \gamma^{+} N\left(P_{1}\right)+E_{q}(x, \xi, t) \bar{N}\left(P_{2}\right) \frac{i \sigma^{+\alpha} \Delta_{\alpha}}{2 M} N\left(P_{1}\right)\right] . \tag{4.6}
\end{align*}
$$

The OPE gives moments in terms of generalized form factors $A_{n, k}(t), B_{n, k}(t), C_{n}(t)$,

$$
\begin{align*}
\int_{-1}^{1} d x x^{n-1} H(x, \xi, t) & =\sum_{\substack{k=0 \\
\text { even }}}^{n-1}(2 \xi)^{k} A_{n, k}(t)+(\mathrm{n}+1 \bmod 2)(2 \xi)^{n} C_{n}(t) \\
\int_{-1}^{1} d x x^{n-1} E(x, \xi, t) & =\sum_{\substack{k=0 \\
\text { even }}}^{n-1}(2 \xi)^{k} B_{n, k}(t)-(\mathrm{n}+1 \bmod 2)(2 \xi)^{n} C_{n}(t), \tag{4.7}
\end{align*}
$$

which can be expressed in terms of local correlators by equations like

$$
\begin{align*}
\left\langle P^{\prime}\right| \bar{q}(0) \gamma^{\left\{\mu_{\mathrm{i}}\right.} D^{\mu_{1}} \ldots \mathrm{i} D^{\left.\mu_{n}\right\}} q(0)|P\rangle & =\bar{U}\left(P^{\prime}\right)\left[\sum _ { i = 0 , e v e n } ^ { n } \left\{\gamma^{\{\mu} \Delta^{\mu_{1}} \ldots \Delta^{\mu_{i}} \bar{P}^{\mu_{i+1}} \ldots \bar{P}^{\left.\mu_{n}\right\}} A_{n+1, i}\left(\Delta^{2}\right)\right.\right. \\
& -\mathrm{i} \frac{\Delta_{\alpha} \sigma^{\alpha\{\mu} \Delta^{\mu_{1}} \ldots \Delta^{\mu_{i}} \bar{P}^{\mu_{i+1}} \ldots \bar{P}^{\left.\mu_{n}\right\}}}{2 m} B_{n+1, i}\left(\Delta^{2}\right) \\
& \left.+\left.\frac{\Delta^{\mu} \ldots \Delta^{\mu_{n}}}{m} C_{n+1,0}\left(\Delta^{2}\right)\right|_{n \text { odd }}\right] U(P) \tag{4.8}
\end{align*}
$$

where $\{\cdots\}$ denotes symmetrization and subtraction of trace terms. The fact that the sum in Eq.(4.7) extends only up to $n-1$ is called polynomiality. The proton alone has eight independent quark GPDs for each quark flavour and typically one can calculate the leading three moments with satisfactory accuracy on the lattice. Adding the gluon GPDs and repeating the analysis for all octet and decuplet baryons and octet mesons one is already speaking about several hundred quantities. In future one will also increasingly analyse hadron resonances and transition form factors, such that the lattice data base will become even richer. For each of these observables one has to analyse the renormalization properties, the quark/pion mass dependence and the finite volume dependence (within suitable versions of effective field theory/chiral perturbation theory (ChPT)). Finally one has to compare results for different lattice actions and analyse the origin of discrepancies. Obviously it is impossible to review all of this here. Rather, we refer to the comprehensive paper 604 for an example of a state of the art analysis. Fig. 4.2, taken from this paper, gives a typical example. This figure shows a number of common aspects:

1. Fluctuations are strongly suppressed for heavy quark/pion masses. This is why the statistical errors (dark blue bars) increase drastically for smalles pion masses.


Figure 4.2. The isosinglet moment $B_{20}^{u+d}(t)$ as a function of simulated pion mass and $t$ [604].


Figure 4.3. Lattice results for $J_{u}$ and $J_{d}$ compared with various models [582, 701, 605, 702 and constraints derived from experiment (colored bands)
2. The difference between the two sheets gives the variation of HBChPT fits. However, it would be safer to only use ensembles with squared pion masses below $m_{\pi}^{2} \leq 0.25 \mathrm{GeV}^{2}$, where ChPT is rather well under control, which was obviously not possible with the ensembles available for this analysis.
3. One is especially interested in the $t=0$ limit of $B_{20}$ in view of Ji's sum rule,

$$
\left\langle J_{q}^{3}\right\rangle=\frac{1}{2}\left[A_{2,0}^{q}(0)+B_{2,0}^{q}(0)\right]
$$

Already today lattice simulations give rather precise results for the total angular momentum carried by the different quark species in a nucleon, see Fig. 4.3. In future these results will further improve, e.g. due to the use of twisted boundary conditions to realize proton momenta different from the natural ones on a lattice, i.e. different from $p_{j}=\frac{2 \pi}{L} n_{j}$.

Thus, much has been done already, and much more will be done in future. Extrapolating the progress of recent years to the time an EIC will start operation it seems realistic to expect


Figure 4.4. An illustration for the transverse probability distribution of the nucleon quark distributions as a function of the transverse quark and nucleon spin direction. Figure taken from 456.
that by then pictures like Fig. 4.2 will be numerically precise and will include reliable error bands.

Another important example are the quark density distributions in the transverse plane plotted in Fig. 4.4. Their form is mainly determined by the Fourier transformations of (moments of) the GPDs.

$$
\begin{align*}
B_{n 0}^{q}\left(x, 0, b_{\perp}^{2}\right) & =\frac{1}{(2 \pi)^{2}} \int_{-1}^{1} d x x^{n-1} \int d^{2} \Delta_{\perp} e^{\mathrm{i} b_{\perp} \cdot \Delta_{\perp}} E\left(x, 0, \Delta_{\perp}^{2}\right) \\
\bar{B}_{T n 0}^{q}\left(x, 0, b_{\perp}^{2}\right) & =\frac{1}{(2 \pi)^{2}} \int_{-1}^{1} d x x^{n-1} \int d^{2} \Delta_{\perp} e^{\mathrm{i} b_{\perp} \cdot \Delta_{\perp}} \bar{E}_{T}\left(x, 0, \Delta_{\perp}^{2}\right) \tag{4.9}
\end{align*}
$$

The information on transverse structure contained in GPDs is, e.g., relevant in the following context: First LHC data show strong disagreement between observed interaction rates and predictions from event generators, see e.g. 703] for the so-called "underlying event" which denotes the whole of all medium hard reaction channels, which are completely dominated by QCD. Part of the explanation might be related to multiple-hard interactions, a class of reactions which was shown to be already relevant at the Tevatron, see [704]. In these reactions multiple hard quark-gluon interactions occur in the same proton-proton collision, which are not described by the usual inclusive factorization theorems. The correction terms have a complicated structure, see e.g. [705] and references cited there, but can be partially related to GPD profiles in the transverse coordinate plane. By combining experimental results from an EIC with improved lattice calculations it should be possible to describe these effects much more precisely than currently. In this context, as always, experimental results are crucial, because it is very difficult to judge the reliability of lattice results without being able to compare with at least some experimental facts.

A multitude of angular asymmetries and hadronic correlations, many of which include spin degrees of freedom, can be measured with a high luminosity EIC. For many of these, the microscopic reaction mechanism is not yet understood. Some of the proposals made depend crucially on the transverse hadronic structure encoded in GPDs, see e.g. [299]. One of the main missions of an EIC is to clarify both the transverse structure and the reaction mechanisms. This is a demanding task which can only be mastered with input from LQCD.

### 4.3 TMDs on the lattice

The availability of methods to study GPDs on the lattice motivates us to develop similar techniques for the calculation of TMDs [279, 280]. In contrast to other, more mature areas of lattice QCD, the present focus of TMD calculations on the lattice is on the development of methodology and on qualitative observations rather than precision. The ultimate goal is to obtain results from first principles only that can potentially be compared to experimental observations. The first step to reach this goal is to describe precisely which matrix elements need to be calculated, and how they can be regularized in the context of TMD factorization. Already at this step, the situation is much more challenging for TMDs than for moments of GPDs, where the matrix elements needed are well-known. These issues are not specific to lattice QCD, but they play a central role in the development of methods to calculate TMDs non-perturbatively.

In its basic form, the correlator that needs to be calculated is that of eq. (2.1). For our purposes, we write the trace projections $\Phi^{[\Gamma]}=\frac{1}{2} \operatorname{Tr}(\Gamma \Phi)$ of this correlator as

$$
\begin{equation*}
\Phi^{[\Gamma]}\left(x, \mathbf{k}_{\perp}\right)=\left.\frac{1}{P^{+}} \underbrace{\int \frac{d(l \cdot P)}{2 \pi} e^{-i(l \cdot P) x}}_{\mathcal{F}_{x}} \underbrace{\int \frac{d^{2} \mathbf{l}_{\perp}}{(2 \pi)^{2}} e^{i 1_{\perp} \cdot \mathbf{k}_{\perp}}}_{\mathcal{F}_{\perp}} \underbrace{\frac{1}{2}\langle P, S| \bar{q}(l) \Gamma \mathcal{W}_{\eta} q(0)|P, S\rangle}_{\widetilde{\Phi}^{[\Gamma]}(l, P, S)}\right|_{l^{+}=0} \tag{4.10}
\end{equation*}
$$

where $\Gamma$ is a Dirac matrix. The gauge $\operatorname{link} \mathcal{W}_{\eta}$ is discussed in sec. 2.4.1, and its geometry is depicted for the SIDIS process in figure 4.5 a). With the generalization of eq. (2.47) it can be written as a concatenation of straight Wilson lines $\mathcal{W}_{\eta}=V_{[l, l+\eta v]} V_{[l+\eta v, \eta v]} V_{[\eta v, 0]}$. Here $v$ is a time-like vector normalized to $v^{2}=1$. A staple shaped gauge link $\mathcal{W}_{\infty}$ extending to $\eta \rightarrow \infty$ corresponds to SIDIS, while a staple $\mathcal{W}_{-\infty}$ directed in the opposite direction corresponds to the Drell-Yan process. Beyond tree level, eq. (4.10) needs to be modified in order to take the collective effect of soft momentum gluons into account and to subtract divergences. This can be achieved, e.g., by dividing $\tilde{\Phi}^{[\Gamma]}$ by appropriate vacuum expectation values (soft factors), see, e.g., [706, 256, 257, [260, 384].

First studies of transverse momentum dependence on the lattice follow the strategy to determine matrix elements of the form $\tilde{\Phi}^{[\Gamma]}$ in eq. (4.10) directly from three-point functions. The idea of using a discrete representation of the non-local operator $\bar{q}(l) \Gamma \mathcal{W}_{\eta} q(0)$ is a novel technique and requires investigations about the properties of such extended operators on the lattice. Considering this and the ambiguities about the precise operator geometry suitable for TMD extraction, it seems reasonable to begin with a simplified setup. The following two operator geometries are under investigation:

- straight gauge link connecting the two quark fields directly, $\mathcal{W}_{0}=V_{[l, 0]}$. This simple setup yields high statistics results, but does not correspond to the situation in SIDIS or Drell-Yan. For example, non-zero time-reversal odd TMDs such as the Sivers function $f_{1 T}^{\perp}$ are forbidden by symmetry with this link geometry. However, the qualitative features of the results are interesting, especially the spin-dependence. A brief outline of findings obtained with straight links is given in sec. 4.3.1
- staple shaped gauge link of finite extent $\mathcal{W}_{\eta}$ for a spacelike choice of the direction $v$ as depicted in figure 4.5 a). Results for the SIDIS link $\mathcal{W}_{+\infty}$ and the Drell-Yan link $\mathcal{W}_{-\infty}$ can be read off if the lattice results converge to a constant for longer and longer staple extents $\eta$. Ongoing studies with this operator geometry are discussed in sec .4.3.2.


Figure 4.5. a) Staple shaped Wilson line. b) Representation of a straight Wilson line (dashed line) as a step-like product of link variables.

### 4.3.1 Straight gauge links

In lattice QCD, it is possible to determine matrix elements $\widetilde{\Phi}^{[\Gamma]}$ appearing in eq. (4.10) directly from a ratio of three- and two-point functions, provided the operator has no extent in Minkowski-time. To do this, we employ the standard methods described in sec. 4.1 Only the operator we insert is specific to our method. Operators with straight gauge links can be approximated on the lattice by a step-like product of link variables, as depicted in figure 4.5 b). At present, disconnected diagrams are neglected. Disconnected diagrams cancel in the isovector channel, i.e., in $u-d$ quark distributions.

The key element to relate the matrix elements $\widetilde{\Phi}^{[\Gamma]}$ determined on the lattice to the TMDs is a parametrization in terms of Lorentz-invariant amplitudes $\widetilde{A}_{i}\left(l^{2}, l \cdot P\right)$, similar to the parametrization in terms of amplitudes $A_{i}\left(k^{2}, k \cdot P\right)$ in ref. [243]. For straight gauge links one obtains

$$
\begin{align*}
\widetilde{\Phi}^{\left[\gamma^{\mu}\right]} & =2 P^{\mu} \tilde{A}_{2}+2 i M^{2} l^{\mu} \widetilde{A}_{3},  \tag{4.11}\\
\widetilde{\Phi}^{\left[\gamma^{\mu} \gamma^{5}\right]} & =-2 M S^{\mu} \widetilde{A}_{6}-2 i M P^{\mu}(l \cdot S) \widetilde{A}_{7}+2 M^{3} l^{\mu}(l \cdot S) \widetilde{A}_{8}, \tag{4.12}
\end{align*}
$$

To translate the amplitudes into TMDs, the Fourier transform in eq. (4.10) must be carried out. For example

$$
\begin{align*}
f_{1}\left(x, \mathbf{k}_{\perp}^{2}\right) & =2 \mathcal{F}_{\perp} \mathcal{F}_{x} \widetilde{A}_{2}\left(l^{2}, l \cdot P\right),  \tag{4.13}\\
g_{1 T}\left(x, \mathbf{k}_{\perp}^{2}\right) & =4 M^{2} \partial_{\mathbf{k}_{\perp}^{2}} \mathcal{F}_{\perp} \mathcal{F}_{x} \widetilde{A}_{7}\left(l^{2}, l \cdot P\right), \tag{4.14}
\end{align*}
$$

where the two independent Fourier transforms $\mathcal{F}_{x}$ and $\mathcal{F}_{\perp}$ are defined in eq. (4.10). On the Euclidean lattice, the matrix elements can only be evaluated in the range

$$
\begin{equation*}
l^{2} \leq 0 \quad|l \cdot P| \leq\left|\mathbf{P}_{\text {lat }}\right| \sqrt{-l^{2}} \tag{4.15}
\end{equation*}
$$

where $\mathbf{P}_{\text {lat }}$ is the three-momentum of the nucleon chosen on the lattice. As a result, data points are only available in a wedge shaped area. The opening angle of the wedge can be potentially increased by using larger lattice nucleon momenta $\mathbf{P}_{\text {lat }}$, but full coverage of the $|l|, l \cdot P$-plane can never be achieved with this method. Thus the information required to reconstruct the $x$-dependence of the distributions is not fully available; the Fourier transform $\mathcal{F}_{x}$ in eqs. (4.13)-(4.14) cannot be carried out. However, model assumptions about the


Figure 4.6. $x$-integrated density of longitudinally polarized quarks inside a nucleon polarized in the transverse $x$-direction. These results have been obtained with straight gauge links at a pion mass $m_{\pi} \approx 500 \mathrm{MeV}$ [279]. The insets display the spin polarization of the quarks and of the nucleon.
correlation of $x$ - and $\mathbf{k}_{\perp}$-dependence can be compared to the lattice data, see sec. VI of ref. [280]. Moreover, the lowest $x$-moment of TMDs can be calculated, since the required information is encoded in the data at $l \cdot P=0$. For example,

$$
\begin{align*}
f_{1}^{[1]}\left(\mathbf{k}_{\perp}^{2}\right) & \equiv \int d x f_{1}\left(x, \mathbf{k}_{\perp}^{2}\right)=\int_{0}^{1} d x\left(f_{1}\left(x, \mathbf{k}_{\perp}^{2}\right)-\bar{f}_{1}\left(x, \mathbf{k}_{\perp}^{2}\right)\right) \\
& =2 \mathcal{F}_{\perp} \widetilde{A}_{2}\left(l^{2}, 0\right), \tag{4.16}
\end{align*}
$$

where $\bar{f}_{1}$ is the unpolarized anti-quark distribution function. First results for the lowest $x$-moments $f_{1}^{[1]}, g_{1 T}^{[1]}$ and $h_{1 L}^{\perp[1]}$ using straight gauge links have been presented in Ref. [279, 280]. The calculations were carried out at a pion mass of about 500 MeV , taking advantage of existing gauge configurations from the MILC collaboration [707] and propagators from the LHP collaboration [708]. The worm gear distribution $g_{1 T}$ gives rise to dipole deformations in the $x$-integrated, $\mathbf{k}_{\perp}$-dependent density of longitudinally polarized quarks inside a transversely polarized nucleon, as shown in figure 4.6. Due to the dipole deformation, this density is not axially symmetric. The peak is clearly shifted away from the center along the axis defined by the transverse spin vector. This shift is associated with a non-zero average transverse quark momentum $\left\langle\mathbf{k}_{x}\right\rangle_{T L}$, which can be expressed in terms of a ratio of amplitudes $\widetilde{A}_{7}(0,0) / \widetilde{A}_{2}(0,0)$. The lattice computations yield $\left\langle\mathbf{k}_{x}\right\rangle_{T L}=67(5) \mathrm{MeV}$ for down quarks and $\left\langle\mathbf{k}_{x}\right\rangle_{T L}=-30(5) \mathrm{MeV}$ for up quarks (errors statistical only). Reference [709] reveals that these results are of the same sign and of quite similar magnitudes as those obtained with a light-cone constituent quark model [409, despite the unphysically large quark masses employed in the lattice calculation.

We note that the straight link results discussed above depend on two additional important ingredients: a non-perturbative renormalization condition and a Gaussian parametrization to perform the Fourier transform, see ref. [280] for details. The renormalization condition is necessary to fix the length-dependent renormalization factor $\exp (-\delta m|l|)$ due to the self-energy of the spacelike Wilson line $\mathcal{V}_{[l, 0]}$ [710, 711, 712]. At the present level of statistical precision, the parametrization of the renormalized data as Gaussian functions is very successful and acts as a provisional regulator of contributions from large $\mathbf{k}_{\perp}$. A better understanding of the operator in the transition from the short range (small $\sqrt{-l^{2}}$, corresponding to large $\mathbf{k}_{\perp}$ ) to the long range behavior may lead to a an improved parametrization of the lattice data, beyond the Gaussian assumption, and may open the possibility to make


Figure 4.7. Test calculation of a T-odd ratio of amplitudes using staple shaped links at $m_{\pi} \approx$ 800 MeV 713 .
contact with a perturbatively defined renormalization scheme.

### 4.3.2 Staple-shaped links and the Sivers function

TMDs obtained with a straight gauge link as discussed in the previous section are not strictly identical to those relevant in, e.g., SIDIS or the Drell-Yan process. Instead, a link geometry as depicted in figure 4.5 a ) is required. In particular, naively time-reversal odd TMD such as the Sivers function can only be non-vanishing once the operator structure involves another direction $v$ related to final or initial state interactions. Lattice QCD can profit from frameworks that avoid rapidity divergences by considering directions $v$ slightly off the lightlike $n^{-}$-direction [240, 241, 256, 257, 260, 384]. TMDs introduced this way follow an evolution equation in the rapidity cutoff parameter $\zeta \equiv(2 P \cdot v)^{2} /\left|v^{2}\right|$ [240, 393]. The restriction to operators $\bar{q}(l) \Gamma \mathcal{W}_{\eta} q(0)$ that have no extent in Euclidean time permits only the implementation of spacelike directions $v$ on the lattice, and furthermore limits the rapidity cutoff parameter to the range $0 \leq \zeta \leq 4\left|\mathbf{P}_{\text {lat }}\right|^{2}$, where $\mathbf{P}_{\text {lat }}$ is the selected nucleon three-momentum on the lattice. The dependence on $v$ leads to additional amplitudes $\tilde{A}_{i}$, $\tilde{B}_{i}$ in the decomposition of the correlator eq. (4.11), compare also [246]:

$$
\begin{align*}
\widetilde{\Phi}^{\left[\gamma^{\mu}\right]}= & \frac{2}{\widetilde{S}}\{ \\
& \left\{P^{\mu} \widetilde{A}_{2}+i M^{2} l^{\mu} \widetilde{A}_{3}+i M \epsilon^{\mu \nu \alpha \beta} P_{\nu} l_{\alpha} S_{\beta} \widetilde{A}_{12}+\frac{M^{2}}{(v \cdot P)} v^{\mu} \widetilde{B}_{1}\right. \\
& +\frac{M}{v \cdot P} \epsilon^{\mu \nu \alpha \beta} P_{\nu} v_{\alpha} S_{\beta} \widetilde{B}_{7}+\frac{i M^{3}}{v \cdot P} \epsilon^{\mu \nu \alpha \beta} l_{\nu} v_{\alpha} S_{\beta} \widetilde{B}_{8}  \tag{4.17}\\
& \left.-\frac{M^{3}}{v \cdot P}(l \cdot S) \epsilon^{\mu \nu \alpha \beta} P_{\nu} l_{\alpha} v_{\beta} \widetilde{B}_{9}+\frac{i M^{3}}{(v \cdot P)^{2}}(v \cdot S) \epsilon^{\mu \nu \alpha \beta} P_{\nu} l_{\alpha} v_{\beta} \widetilde{B}_{10}\right\} .
\end{align*}
$$

Here $\widetilde{S}$ generically represents a soft factor modification, as needed, e.g., in the formalism of refs. [256, 257, 260, 384]. First lattice studies are ongoing for ratios of amplitudes, in which renormalization factors and potential soft factors cancel [713, 280], similar as in the asymmetries discussed in sec. 2.2.7. Figure 4.7 shows results from a test calculation [713] of a ratio of time-reversal odd over time-reversal even amplitudes $R_{\text {odd }} \equiv\left(\widetilde{A}_{12}-\right.$ $\left.\left(M /\left|{\underset{\sim}{\mathbf{P}}}_{\text {lat }}\right|\right)^{2} \widetilde{B}_{8}\right) / \widetilde{A}_{2}$, evaluated at $l \cdot P=0,\left|\mathbf{P}_{\text {lat }}\right| \approx 0.5 \mathrm{GeV}$, for selected values of $l^{2}$. Note that $\widetilde{A}_{12}$ would correspond to the Sivers function $f_{1 T}^{\perp}$ for lightlike $v$. In the test calculation, the operator has been evaluated with staple shaped links $\mathcal{W}_{\eta}$ for a large range of extents $\eta$.

The result of the test calculation is, within statistics, an odd function of $\eta v \cdot P$, as expected for a time-reversal odd function. Moreover, we see the onset of a plateau at $|\eta v \cdot P| \gtrsim 2$. The plateau at large positive $\eta$ correspond to the SIDIS result with a $\mathcal{W}_{\infty}$ link, while the plateau at large negative $\eta$ correspond to the Drell-Yan result with the $\mathcal{W}_{-\infty}$ link. This is a promising indication that lattice estimates could be feasible for, e.g., the average transverse momentum shift due to the Sivers function given by

$$
\begin{equation*}
\left.\left\langle\mathbf{k}_{y}\right\rangle_{T U} \equiv \frac{\int d^{2} \mathbf{k}_{\perp} \mathbf{k}_{y} \Phi^{\left[\gamma^{+}\right]}}{\int d^{2} \mathbf{k}_{\perp} \Phi^{\left[\gamma^{+}\right]}}\right|_{\mathbf{S}_{\perp=(1,0)}}=M \frac{\int d x f_{1 T}^{\perp(1)}(x)}{\int d x f_{1}^{(0)}(x)}, \tag{4.18}
\end{equation*}
$$

see also [264, 444. Here $\Phi^{\left[\gamma^{+}\right]}$intuitively has an interpretation as the density of unpolarized quarks in a transversely polarized proton, and $f_{1 T}^{\perp(1)}$ and $f_{1}^{(0)}(x)$ are $\mathbf{k}_{\perp}$-moments defined as $f^{(n)}(x) \equiv \int d^{2} \mathbf{k}_{\perp}\left(\mathbf{k}_{\perp}^{2} / 2 M^{2}\right)^{n} f\left(x, \mathbf{k}_{\perp}^{2}\right)$. A generalized version of the above quantity can be formed directly from the amplitudes determined on the lattice, namely

$$
\begin{equation*}
\left\langle\mathbf{k}_{y}\right\rangle_{T U}\left(\mathcal{B}_{\perp}\right) \equiv M \frac{\int d x \tilde{f}_{1 T}^{\perp(1)}\left(x, \mathcal{B}_{\perp}^{2}\right)}{\int d x \tilde{f}_{1}\left(x, \mathcal{B}_{\perp}^{2}\right)}=-\left.M \frac{\widetilde{A}_{12}-R(\zeta) \widetilde{B}_{8}}{\widetilde{A}_{2}+R(\zeta) \widetilde{B}_{1}}\right|_{l \cdot P=0} ^{l^{2}=-\mathcal{B}_{\perp}^{2}} \tag{4.19}
\end{equation*}
$$

with $R(\zeta)=1-\sqrt{1+4 M^{2} / \zeta}$ and where $\tilde{f}_{1}$ and $\tilde{f}_{1 T}^{\perp(1)}$ are now $\mathbf{k}_{\perp}$-Fourier-transformed TMDs as they appear in eq. (2.33). Keeping the length $\mathcal{B}_{\perp}$ sufficiently large compared to the lattice spacing and correspondingly assuming renormalization properties as in continuum field theory, one finds that multiplicative renormalization factors, including Wilson line self-energies, as well as potential soft factors cancel in the ratio of amplitudes above. The extrapolation to $\mathcal{B}_{\perp}=0$, where $\left\langle\mathbf{k}_{y}\right\rangle_{T U}\left(\mathcal{B}_{\perp}\right)$ is equal to $\left\langle\mathbf{k}_{y}\right\rangle_{T U}$, will require special attention to UV divergences and cutoff effects. However, already the generalized object $\left\langle\mathbf{k}_{y}\right\rangle_{T U}\left(\mathcal{B}_{\perp}\right)$ at nonzero $\mathcal{B}_{\perp}$ may offer opportunities to compare with phenomenology, by means of an $x$-integrated version of the Bessel-weighted quantities introduced in eq. (2.33) A possible difficulty for lattice computations will be to reach large enough values $\zeta$, in the regime where evolution equations [240, 393] can be applied.

### 4.4 Spectroscopy and other physics topics

Still another approach to elucidate hadron structure is offered by lattice spectroscopy. Spectroscopy has the great advantage that it allows to avoid the subtle renormalization issues mentioned above, but the disadvantage that the deduction of information on hadron structure is less direct. A typical recent example is found in [714], see Fig. 4.8. The basic idea is that one uses a set of interpolating currents (sources) $\mathcal{O}_{i}$ with the same quantum numbers to calculate and analyse the correlation matrix as a function of separation of the time-hyper planes

$$
\begin{equation*}
C_{i j}(t)=\langle 0| \mathcal{O}_{i}(t) \mathcal{O}_{j}(0)|0\rangle \tag{4.20}
\end{equation*}
$$

and solves the generalized eigenvalue problem. One thus obtains not only the eigenvalues (masses) but also the eigenvectors in terms of the different sources. If done with care the relative overlap of the physical mass states with the different sources allows to draw conclusions about their structure. This provides information, which is often complementary to that obtained with the methods sketched above. Again for practical purposes this information is most sensitive to leading Fock-state components. While this is a very powerful method, its results must be interpreted with care. The eigenvectors of different mass states give the amplitudes with which each source contributes. All of these are forced to be orthonormal by construction. This constraint can lead to substantial artifacts if the chosen source functions span too small a function space. To avoid premature conclusions one, therefore, has to compare results obtained for different lattice actions and many different choices of sources. Presently the lattice community is still in the process of optimizing this method, but it seems already clear by now that in a few years this approach will be a standard source of many detailed information about hadron structure.


Figure 4.8. A typical example from [714]. The $1^{-}$kaon states are shown. Color coding indicates dominance of a particular charge-conjugation eigenstate

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## Chapter 5

## QCD matter under extreme conditions

Convenors and chapter editors:
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### 5.1 Chapter summary: overview and golden measurements

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A basic quest of nuclear physics is the understanding of the structure of hadrons and nuclei (nucleon number $A>1$ ) in terms of QCD Lagrangian degrees of freedom, the quarks and gluons. Deviations of the nuclear quark and gluon densities from the sum of the free nucleon densities directly attest to binding effects and elucidate the QCD origin of the inter-nucleon interactions. Such deviations can arise through different mechanisms, such as a modification of the free nucleon structure, the presence of non-nucleonic degrees of freedom, and quantum-mechanical interference of the quark/gluon fields of different nucleons at small parton fractional momentum $x$ ("shadowing"), creating a fascinating landscape of many-body QCD. At even smaller $x$, the gluon density increases to the point where gluons become closely packed, leading to a strong field regime of non-linear QCD evolution called saturation. This regime is argued to have universal properties for any hadronic system, ranging from pions, to protons and nuclei, but its onset is enhanced in nuclear targets due to the superposition of the gluon field of many nucleons.

A peculiar pattern of nuclear modifications was observed in fixed-target experiments and caused much excitement; it shows suppression for $0.2<x<0.8$ ("EMC effect"), some signs of enhancement for $0.05<x<0.2$, and significant suppression (shadowing) at smaller $x$. However, such experiments were unable to reach deep into the shadowing region or probe gluons. The EIC will overcome these limitations, extend measurements to very high scales of $Q^{2}$, and determine with high precision the nuclear effects on gluon distributions. Full reconstruction of the hadronic final state also opens up for the first time the possibility of measuring charged current interactions on nuclei, and to perform a full quark flavour separation based on nuclear DIS data only. Crucially, an EIC will access much lower values of $x<0.01$ and study the onset of the saturation regime, which has never been directly probed experimentally, although tantalising (but not unequivocal) signatures have been found at the Relativistic Heavy-Ion Collider (RHIC).

Another possibility offered by nuclear targets is the study of the propagation of colour charges in nuclear matter and the space-time evolution of hadronization. The unique feature of an EIC, compared to previous fixed target experiments, is its large energy span. This allows one to experimentally boost hadronization effects completely out of the nucleus, in order to focus attention on the propagation of fast quarks and gluons, and their accompanying parton showers, through the nucleus. Thus one can use the partons as coloured probes of the soft components of the target nuclear wave function, and conversely experimentally test QCD mechanisms of parton energy loss in a known nuclear medium. At lower energies, hadronization happens partially inside the nucleus, which can then be used as a femtometer scale detector of the process. A good control of energy loss mechanisms in the partonic phase will yield unambiguous insights into the dynamics of colour confinement whereby hadrons emerge from coloured quarks and gluons.

Novel observables will be available thanks to the high energy reach, namely heavy flavours, charmonium and bottomonium, and jets, greatly expanding the experimental toolbox and sensitivity to nuclear effects, and thereby allowing a close connection to first principles calculations in QCD. The collider mode will also make it feasible to study in detail target fragmentation and its correlation to current fragmentation through multi-particle correlations, thereby expanding considerably the study of shower development and hadronization mechanisms.

### 5.1.1 Gold and silver measurements

One of the goals of the program at the INT was to identify a small number of measurements whose ability to extract novel physics is beyond question and which are feasible at an EIC. Such measurements are referred to as "golden" measurements. These are complemented by other "silver" measurements/observables, to form a broad, robust, and compelling physics program. The gold and silver measurements are summarised in Tables 5.1 and 5.2, where also their feasibility in phase-I (medium energy) and phase-II (full energy) is indicated, and further discussed below. Many more observables than can fit in this section will be available at an EIC, contributing to a very rich physics program exploring the QCD basis of nuclear physics. Many of these will be reviewed in detail in the rest of this chapter.

| Deliverables | Observables | What we learn | Phase-I | Phase-II |
| :---: | :---: | :---: | :---: | :---: |
| integrated gluon | $F_{2, L}$ | nuclear wave.fn.; <br> saturation, $Q_{s}$ | gluons at <br> $10^{-3} \lesssim x \lesssim 1$ | explore sat. <br> regime |
| $k_{T}$-dep. gluons; <br> gluon correlations | di-hadron <br> correlations | non-linear QCD <br> evolution/universality | onset of <br> saturation; $Q_{s}$ | RG evolution |
| transp. coefficients <br> in cold matter | large- $x$ SIDIS; <br> jets | parton energy loss, <br> shower evolution; <br> energy loss mech. | light flavours, charm <br> bottom; jets | precision rare <br> probes; <br> large- $x$ gluons |

Table 5.1. Golden measurements in $e+A$ collisions at an EIC

| Deliverables | Observables | What we learn | Phase-I | Phase-II |
| :---: | :---: | :---: | :---: | :---: |
| integrated gluon <br> distributions | $F_{2, L}^{c}, F_{2, L}^{D}$ | nuclear w.fn.; <br> saturation, $Q_{s}$ | early sat. onset <br> challenge to measure | saturation <br> regime |
| flavour separated <br> nuclear PDFs | charged current <br> $\& \gamma Z$ str. fns. | EMC effect origin | full $q_{i}$ separation <br> at $0.01 \lesssim x \lesssim 1$ | larger $Q^{2}$, <br> smaller $x$ |
| $k_{T}$-dep. gluons | SIDIS at <br> small- $x$ | non-linear QCD <br> evolution/universality | extract $Q_{s} ;$ <br> multipole corr. | RG evol.; <br> flavour sep. |
| $b$-dep. gluons; <br> gluon correlations | DVCS; <br> diffractive $J / \Psi$, <br> \& vector mesons | interplay between <br> small- $x$ evolution <br> and confinement | moderate $x$ with <br> light, heavy nuclei | smaller $x$, <br> saturation |

Table 5.2. Silver measurements in $e+A$ collisions at an EIC

### 5.1.2 QCD at high gluon density

The fact that we do not know the dynamics of gluons in nuclei over basically any $x$ range seems a compelling enough reason to build an EIC. The non-Abelian nature of QCD is its most distinguishing feature and controls emergent phenomena such as colour confinement, chiral symmetry breaking and the generation of the vast bulk of the visible mass in the Universe. These are, however, non-perturbative phenomena which are difficult to attack from first principles; where this is possible, such as in the case of the hadron spectrum from lattice QCD, only static aspects of the strong interactions are addressed. An EIC would allow one for the first time to experimentally probe at small $x$ dynamical non-Abelian aspects of a fundamental force of nature in a controlled setting where weak coupling methods apply. The physics in this regime is the non-perturbative physics of strong


Figure 5.1. The saturation scale, $Q \equiv Q_{s}$, and how it scales with $x$, and $A$.
colour fields; the important new feature is that the applicability of weak coupling methods allow for systematic comparisons of theory to experiment.

In addition to the intrinsic interest in this novel many-body regime of QCD, experimentally establishing and refining an effective field theory for the saturation regime - such as the Colour Glass Condensate (CGC) - as well as precisely imaging the distribution and correlations of small- $x$ partons in nuclei, besides being of intrinsic interest, would have wide-ranging applications. The universality of the saturation regime implies that such a theory would provide a microscopic basis for understanding and calculating total hadronic cross sections, with important applications to, for example, ultra-high energy cosmic ray physics, where extrapolations in energy of several orders of magnitude are required to compute their spectrum and detect possible new physics effects. In high-energy relativistic heavy-ion collisions, the release of saturated low- $x$ partons represents the starting point of the subsequent space-time evolution of the Quark-Gluon Plasma (QGP). Testing and benchmarking the underlying theory opens the prospect of a controlled, and precise, first principles calculation of such an initial state. Thereby reducing one of the largest sources of uncertainty in the interpretation of experimental observables, and the measurements of the QGP properties: an EIC would offer to the RHIC and LHC heavy-ion programs an important asset, as valuable as the one HERA provided to the LHC p+p program.

The onset of the saturation regime, when the gluon density becomes so large that further growth with energy is tamed, is characterised by the saturation scale $Q_{s}(x)$; partons with momenta below this scale overlap in transverse space, so that parton recombination and screening stops further growth in their number density. Given that parton distributions grow as $x$ decreases, and dramatically so as discovered at HERA, the saturation scale is clearly expected to grow as $x$ decreases. It is further enhanced in nuclear targets because of the overlap of the gluon fields originating from different nucleons. This is illustrated in figure 5.1. In the saturated, dense regime at small $x$, non-linear QCD dynamics becomes dominant but at the scale being set by a semi-hard $Q_{s}$ (of order 1 GeV ), calculations can be carried out by weak coupling techniques and suitable effective field theories, of which the CGC is a prime example, can be derived from first principles.

The dilute-dense separation of scales is more subtle than just described. The larger
the gluon's transverse momentum $k_{T}$, the smaller its longitudinal energy fraction $x$ needs to be to enter the saturation regime. In a scattering process, dilute partons (with $k_{T} \gg$ $\left.Q_{s}(x)\right)$ behave incoherently, whilst when the parton density is large $\left(k_{T} \lesssim Q_{s}(x)\right)$, gluons scatter coherently. Therefore, transverse momentum dependent observables will be able to uncover more details than inclusive observables, which can only access averaged saturation effects. The interplay of saturation and the transverse spatial distribution of gluons is also important; as $x$ decreases, gluon densities saturate first in the centre of the nucleus. To accommodate further growth, gluons will be pushed more and more to the periphery, so that the average gluon radius is expected to increase with decreasing $x$.

For all these reasons regarding the small- $x$ physics program in $\mathrm{e}+\mathrm{A}$ collisions, the physics deliverables of an EIC have been classified in three main categories giving access to the integrated, transverse-momentum-dependent, and impact-parameter-dependent gluons. Here, by "gluons" we mean not only the conventional single-gluon distributions but also multigluon correlations. These have often been of secondary interest, but are now recognised as essential to a full understanding of the low- $x$ regime. Indeed, except for the most inclusive observables which are subject to cancellations, consistent QCD calculations in the nonlinear regime require the knowledge of multi-gluon distributions. Integrated, transverse-momentum-dependent, and impact-parameter-dependent gluon distributions and correlations in nuclei are all unknown, and the processes we discuss below have never been measured at small $x$.

## Integrated gluons and sea-quarks

As the most basic observables from both the theory and experimental sides, the inclusive $(e+\mathrm{A} \rightarrow e+\mathrm{X})$ structure functions $F_{2}$ and $F_{L}$ stood out among other measurements, already well before the INT programme. They were the first potential golden measurements discussed; the pros and cons of these candidates to pin down the gluon and sea-quark distributions in nuclei were further reviewed during the program.
$F_{2}$ is the most inclusive observable in deep inelastic scattering. Its measurement presents no particular experimental challenge. On the theory side, it is the simplest process to calculate, along with $F_{L}$, with the fewest input assumptions. For instance, $F_{2}$ and $F_{L}$ will be the first observables for which a full NLO calculation in QCD including non-linear effects will be available. (The existing phenomenology is still based on leading-order "impact factor" computations.)

Although it is harder to extract experimentally, $F_{L}$ is a golden measurement for high density QCD because it is more directly related to the gluon distribution. Furthermore, it is more sensitive to non-linear effects than $F_{2}$. In the latter, higher-twist contributions cancel each other out delaying the onset of non-linear effects. The necessity of performing an energy scan to measure $F_{L}$ implies that the accessible $x$ range is a bit smaller than accessible with the $F_{2}$ measurement. However, the increased sensitivity to non-linear effects more than compensates for this shortcoming. Deviations of DGLAP fits of the simultaneous "singlet" dominated (at small $x$ ) evolution of $F_{2}$ and $F_{L}$ determined from EIC data should be able to quantitatively determine the onset of the saturation regime. The case for the low-energy EIC needs to be investigated more; in particular, the implementation of non-linear effects must be made more accurate, and more detailed DGLAP fits of EIC pseudo-data should be performed before establishing its sensitivity to saturation physics in the inclusive channel. One caveat discussed is that QED radiative corrections for nuclear targets can be large, and it remains to be proven that they can be controlled to the required precision. Computations
addressing the role of these radiative corrections are underway and are discussed further in the detector studies section of this report.

The charm structure functions $F_{2, L}^{c}$ were considered as silver measurements for the nonlinear regime. As in the case of $F_{L}$, these observables give more direct access to the gluon distribution relative to $F_{2}$; however due to the mass of the charm quark, they also probe higher values of $x$ and are therefore less sensitive to non-linear effects. In addition, QCD calculations with non-zero charm mass are scheme dependent, which can absorb signals of non-linear effects if not appropriately handled. However, since they can be measured precisely with a properly-designed vertex detector, charm structure functions will be a very important complementary measurement to pin down the nuclear gluon distribution throughout the $\left(x, Q^{2}\right)$ plane.

Last but not least, silver measurements in the inclusive category are those of the diffractive structure functions $F_{2}^{D}$ and $F_{L, D}$. These are sensitive to the square of the gluon distribution. As may therefore be anticipated, the strongest hints for manifestations of non-linear effects in $\mathrm{e}+\mathrm{p}$ collisions at HERA come from diffractive measurements. A striking example is the fact that the ratio of the diffractive to inclusive structure function is constant with energy, an observation not easily reconciled in a leading twist scenario. Furthermore, the leading-twist approximation does not explain the geometric scaling of the diffractive cross section. Finally, as a sign of enhanced sensitivity to non-linear effects, the DGLAP analysis of diffractive structure functions from HERA is problematic at larger values of $Q^{2}$ relative to the same for $F_{2}\left(\sim 8 \mathrm{GeV}^{2}\right.$ in the former compared to $2 \mathrm{GeV}^{2}$ in the latter). However, measurements of diffractive structure functions are relatively more difficult and the additional kinematic variables make the analyses more involved than for $F_{2, L}$.

## Transverse momentum dependent gluons and sea-quarks

The golden measurement here is that of di-hadron azimuthal correlations in $e+\mathrm{A} \rightarrow$ $e+\mathrm{h}_{1}+\mathrm{h}_{2}+\mathrm{X}$ processes. Di-hadron correlations are not only sensitive to the $k_{T}$ dependence of the gluon distribution but also to the $k_{T}$ dependence of gluon correlations. These correlations are sensitive to multi-gluon distributions for which first principles computations are only now becoming available. Precise measurements of these di-hadron correlations at an EIC would allow one to extract these multi-gluon correlations and study their non-linear evolution. Saturation effects in this channel correspond to a progressive disappearance with decreasing $x$ of the peak in the di-hadron azimuthal angle difference around $\Delta \phi=\pi$. In a leading twist picture, where there is only one hard scattering, one expects, from momentum conservation, that the peak will persist. A comparison of the heights and widths of the dihadron azimuthal distributions in $e+\mathrm{A}$ and $e+\mathrm{p}$ collisions respectively would clearly mark out such an effect experimentally. An analogous phenomenon has already been observed for di-hadrons produced at forward rapidity in $\mathrm{d}+\mathrm{Au}$ and $\mathrm{p}+\mathrm{p}$ collisions at RHIC. In that case, di-hadron production proceeds from valence quarks in the deuteron (proton) scattering on small- $x$ gluons in the target Au nucleons (proton), $q_{V}+\mathrm{Au}(\mathrm{p}) \rightarrow \mathrm{h}_{1}+\mathrm{h}_{2}+\mathrm{X}$. Lacking direct experimental control over $x$, the onset of the saturation regime is controlled by changing the centrality of the collision, the di-hadron rapidity and the transverse momenta of the produced particles. Experimentally, a striking flattening of the $\Delta \phi$ peak in $\mathrm{d}+\mathrm{Au}$ collisions is observed in central collisions, but the peak reappears in peripheral collisions or for mid-rapidity di-hadrons. Directly using a point-like electron probe, as opposed to a quark bound in a proton or deuteron, is extremely beneficial. It is experimentally much cleaner as there is no "spectator" background to subtract and the access to the exact kinematics of
the process allows for more accurate extraction of the physics than is possible at RHIC or in the future with $\mathrm{p}+\mathrm{A}$ collisions at the LHC. Because there is such a clear correspondence between the physics of this particular final state in $\mathrm{e}+\mathrm{A}$ collisions to the same in $\mathrm{p}+\mathrm{A}$ collisions, this measurement is an excellent testing ground for quantitative studies of the universality of multi-gluon correlations in $\mathrm{p}+\mathrm{A}$ and $\mathrm{e}+\mathrm{A}$ collisions.

The simplest process to extract the transverse momentum dependence of the gluon distribution is single inclusive DIS (SIDIS), $e+\mathrm{A} \rightarrow e+\mathrm{h}+\mathrm{X}$. One reason why these processes are especially interesting is that by having two momentum scales at one's disposal, it is possible to keep $Q^{2}$ large and access the saturation regime at transverse momenta $p_{T} \lesssim Q_{s}$. This way, non-perturbative effects and higher-twist contributions are suppressed, but one can nonetheless access non-linear QCD dynamics. Considering that $Q_{s}$ will not exceed a few GeV at an EIC, this helps one disentangle strong coupling effects, characterized by a fixed scale ( $\Lambda_{Q C D}$ ), from weak coupling non-linear effects more cleanly relative to inclusive observables. Furthermore, in the large $Q^{2}$ and small $x$ limits, the relation between the transverse momentum of the produced hadron $p_{T}$ and that of the small-x glue $k_{T}$ is quite direct, enabling a rather straightforward experimental probe of the gluon transverse momentum distribution. From the theoretical point of view, important connections have been established between the framework of Transverse Momentum Dependent (TMD) distributions discussed previously in this report and the CGC effective theory at small $x$. Thus SIDIS has all the pre-requisites to be considered a golden observable. It is nonetheless classified as silver because di-hadron correlations are more directly sensitive to non-linear QCD evolution.

## Transverse position dependence of gluons and sea-quarks

To pin down the transverse distribution and correlations of small- $x$ gluons, exclusive measurements are needed. The prototypical observables discussed are diffractive vector meson production (DVMP) and deeply virtual Compton scattering (DVCS). Coherent diffraction, where the nuclear target is intact, gives access to the transverse spatial distribution of the gluon density in a nucleus. Incoherent diffraction, where the nuclear target breaks up, but is separated by a rapidity gap from the projectile fragmentation region, allows one to extract, in addition, transverse plane correlations. These shed important light on the spatial picture of the partonic sub-structure of nuclei. In addition, both contribute crucial information necessary to understand the spatial gluon distributions that form the initial conditions for heavy ion collisions. $J / \Psi$ meson production off nuclei is the most widely considered exclusive channel; those of other vector mesons $\rho, \phi$ ) provide important complementary information. DVCS, though luminosity hungry, is free of the uncertainty from incomplete knowledge of vector meson wave-functions.

Coherent diffractive $J / \Psi$ production has been extensively discussed as potentially the golden measurement in this category. However, while the physics goals are golden, the technical challenges are formidable. Coherent diffraction dominates over incoherent diffraction only at rather low values of $t$. It was determined that a rejection of the target-dissociation background with at least $95 \%$ efficiency is required in order to measure the coherent cross section up to large enough momentum transfers, and a 20 MeV resolution on the momentum transfer is also needed in order to extract precise enough information in impact parameter space. While this measurement is more feasible in light nuclei, it becomes more challenging in heavier nuclei. For light nuclei, coherent diffraction could shed important light on short range nuclear forces. For larger nuclei, it is unclear at present whether what one learns is
distinguishable from the distribution of gluons obtained from the Woods-Saxon distribution of nucleons in the nucleus; the ability for coherent diffraction to distinguish between different dynamical models for large nuclei is disputed. For these reasons, it is classed as a silver measurement.

Studies of the incoherent regime of diffractive vector meson production are slowly but surely emerging. This process is a priori more sensitive to high parton densities than is coherent diffraction. This is because it is much easier to measure at large $t$, corresponding to small values of $b$, nearer the center of the nucleus where the gluon density is the largest. However, the amount of information that can be extracted from nuclear fragments is not clear, since the theoretical description of the nuclear break-up remains a challenge. The minimum requirement is to be able to identify if the nucleus breaks up into its constituent nucleons or if the nucleons themselves break-up, as the corresponding calculations require different theoretical tools. Neither experimental or theoretical works on this process are mature enough to classify it as a golden measurement. However, the effects predicted by saturation models are large and unique enough that an observation of these will be convincing evidence of this physics. Therefore, both theoretical and experimental studies of this channel should be pursued vigorously.

### 5.1.3 Parton substructure of nuclei

Nuclear deep-inelastic scattering with an EIC will provide a unique measurement of gluon and sea quark densities in the "dilute" regime at $x \gtrsim 0.01$ in a range of nuclei. While the quark densities in the region $0.05 \lesssim x \lesssim 0.6$ were studied in fixed target experiments and will be further explored at JLab with 12 GeV electron beams, the behaviour of the gluon and sea quark densities in this region is essentially unknown. An EIC will have sufficient coverage in $Q^{2}$ to extract the nuclear gluon density through the $Q^{2}$ dependence of the nuclear structure function $F_{2}^{A}$. Furthermore, direct access to gluons can be gained from the longitudinal structure function $F_{L}^{A}$ through measurements at different beam energies, or additionally, by tagging charm production.

A reliable determination of the nuclear gluon density in the dilute regime is essential for a quantitative assessment of the onset of the new QCD regime of high parton densities and non-linear gluon interactions, which will be more widely accessible at a full-energy EIC. At $x \gtrsim 0.1$, an EIC will also explore gluon anti-shadowing and EMC effects - a step that might prove as revolutionary for our understanding of nuclei as the discovery of the quark EMC effect 30 years ago. For these reasons, inclusive $F_{2, L}$ structure function measurements at larger $x$ complement those discussed for the small- $x$ regime.

As it turns out, the high luminosity envisaged for an EIC enables measurements of nuclear electromagnetic structure functions up to $x \approx 1$ competitively with, or even surpassing, what has been achieved to date in fixed target experiments. (Since the maximum $x$ in a nucleus is $A$, collider high luminosity measurements could uncover interesting physics in the Fermi regime where partons carry more more momenta than a bound nucleon.) Furthermore, the large $Q^{2}$ range and hadronic event reconstruction capabilities will also likely allow measurement of charged current structure functions, and possibly of $\gamma-Z$ interference structure functions. See the chapter on electroweak physics for further discussion. This will enable full quark flavour separation utilising only nuclear DIS data, and offer, for example, new handles on the origin of the EMC effect such as its flavour dependence. In this context, one should also mention the possibility of extracting information on particular twist four operators, which play an important role in parity violating DIS in the EMC region.

These measurements are highly interesting, important, and in some cases unique to an EIC compared to previous facilities. However, more work is needed to establish to what extent full flavour separation can be effectively carried out at an EIC; we therefore classify them as silver measurements.

Much more information on the nuclear modification of the quark/gluon structure of the proton and neutron can be gained from deep-inelastic measurements with detection of the spectator system of $(A-1)$ nucleons in the final state. In particular, measurements on deuterium with a spectator proton can measure structure functions of the bound neutron ranging from nearly on-shell to far off-shell, facilitating the extrapolation to an on-shell neutron. Measurements with a spectator neutron, which are extremely difficult with a fixed target but feasible at a collider using a zero degree calorimeter, provide completely new information on the off-shell proton structure functions, and constrain theoretical models by comparison to the well known free proton wave function. With heavier nuclear targets, one could explore the effects of parton/nucleon embedding in a complex nuclear environment. While no technical difficulty is foreseen, detailed studies of the required detectors are needed to determine the feasibility and precision of these measurements.

### 5.1.4 Parton propagation and hadronization in nuclear matter

The transition from coloured partons (quarks and gluons) to colourless hadrons - the so-called hadronization or fragmentation process - exemplifies a fundamental process in QCD which still lacks a quantitative understanding from first principles calculations. Fragmentation functions, which encode the probability that a parton fragments into a hadron, have been obtained by fitting experimental data covering large kinematic ranges and numerous hadron species. However, knowledge about the dynamics of the process remains limited and model dependent. A particular model, see figure 5.2, posits a separation of scales between a short time scale for colour neutralization due to confinement generating a colourless "pre-hadron" and a longer time scale (presumably controlled by chiral symmetry breaking), which governs the formation of hadrons. The dynamical consequences of such a model are distinguishable from other models where the separation of scales is reversed or is non-existent. Extracting these time scales would be an important step towards understanding how hadrons emerge dynamically from partons, complementing the information on properties of colour confinement extracted from lattice measurements of ground state "static" correlators.

Nuclear deep inelastic scattering (nDIS) provides a known and stable nuclear medium ("cold QCD matter") and a final state with strong experimental control on the kinematics of the hard scattering. This permits one to use nuclei as femtometer-scale detectors of the hadronization process, see figure 5.2. In fact, both the energy loss due to medium-induced gluon bremsstrahlung off a quasi-free parton and the pre-hadron re-interaction with the surrounding nucleons lead to attenuation and transverse momentum broadening of hadron yields compared to proton targets, and allow experimental access to the space-time evolution of hadronization. Theoretical models of this process can be calibrated in nDIS and then applied, for example, to the study of the Quark-Gluon Plasma ("hot QCD matter") created in high-energy nucleus-nucleus collisions.

The combination of high energy and luminosity offered by an EIC promises a truly qualitative advance in this field, compared with current and planned fixed target experiments. The large $Q^{2}$ range permits measurements in the fully calculable perturbative regime with enough leverage to determine nuclear modifications in the QCD evolution of


Figure 5.2. Parton propagation and hadronization in cold and hot nuclear matter. A scenario of possibly distinct colour neutralization $\left(t_{C N}\right)$ and hadron formation $\left(t_{F}\right)$ time scales is illustrated on the vertical time axis.
fragmentation functions; the high-luminosity permits the multidimensional binning necessary for separating the many competing effects and for detecting rare hadrons. The large $\nu$ range ( $\approx 10-1000 \mathrm{GeV}$ ) allows one to experimentally boost the hadronization process in and out of the nuclear medium, in order to isolate in-medium parton propagation effects (large $\nu$ ) and cleanly extract colour neutralization and hadron formation times (small $\nu$ ); furthermore, using the quark flavour separated nuclear PDFs expected from an EIC, one could analyze nuclear Drell-Yan data, which are free from hadronization effects, and isolate initial state parton energy loss from nuclear wave function effects, enabling a complete experimental study of colour charge interactions in cold nuclear matter. For the first time, one will be able to study hadronization of open charm and open bottom meson production in $e+A$ collisions, as well as the in-medium propagation of the associated heavy quarks: these allow one to fundamentally test high-energy QCD predictions for energy loss, and confront puzzling measurements of heavy flavour suppression in the Quark-Gluon Plasma at RHIC. Within a collider environment, one would also be able to separate target from current hadronization and cross-correlate these two, adding a new dimension to hadronization studies.

The scattered quarks and gluons, from which the final-state hadrons emerge, couple to other nuclear gluons. Good control over the colour neutralization time scale will allow one to use this internally created colour radiation to explore the structure of nuclear matter in close analogy with the well-known exploration of matter with electromagnetic radiation or electrically charged particles. Furthermore, an EIC with $\sqrt{ } s \gtrsim 30 \mathrm{GeV}$ will permit for the first time the measurement of jets and their substructure in $e+\mathrm{A}$ collisions, furnishing a novel and extensive set of observables which directly access quark energy loss and the as yet untested parton shower mechanism, fundamentally described in QCD and pervasive in applications to particle physics simulations. Jet nuclear modifications can also be directly related to the propagation of the coloured partons shower in the nuclear medium, and used to measure the cold nuclear matter transport coefficients which encode basic information on the non-perturbative soft gluon structure of the nuclei. These measurements are complementary to direct inclusive and diffractive structure functions measurements at small $x$ in accessing the high-density non-linear QCD regime, but are entirely feasible with a low-energy EIC.

The outlined parton propagation and hadronization program can for the most part be carried out in phase-I. In phase-II, we do not anticipate any qualitative new lesson will be
learned, while the increased energy and $Q^{2}$ range may prove useful, for instance, for more refined studies in the jet and heavy flavour sectors, and offering an increased reach towards small $x$ for nuclear gluon measurements via $2+1$ jet production.

In conclusion, due to the physics interest, theoretical interpretability and feasibility in phase-I, this jet and heavy quark study program as a whole was classified as a golden measurement for $e+\mathrm{A}$ collisions at an EIC, with light quark SIDIS classified as a silver measurement.

### 5.2 Review of linear and non-linear approaches in QCD at small-x

## Collinear factorization and DGLAP evolution

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The evaluation of strong interaction cross-sections which involve hard scales is possible thanks to QCD factorization theorems. The latter are derived from first principles in QCD [716, 717] and allow the factorization of cross sections into hard scattering coefficients (computed in a perturbative expansion in the strong coupling constant) and parton densities which contain information about nonperturbative dynamics. Parton densities, due to their intrinsically non-perturbative nature, cannot be directly evaluated from first-principles lattice computations except perhaps in very limited kinematic windows. Nevertheless, their evolution with hard scale can be calculated. This is done usually using the renormalization group DGLAP equations,

$$
\begin{equation*}
\mu \frac{d}{d \mu} f_{j / h}(x, \mu)=\sum_{k} \int_{x}^{1} \frac{d z}{z} P_{j k}\left(z, \alpha_{s}(\mu)\right) f_{k / h}(x / z, \mu), \tag{5.1}
\end{equation*}
$$

with the splitting functions which have perturbative expansion in powers of the strong coupling constant $\alpha_{s}$,

$$
\begin{equation*}
P_{j k}\left(z, \alpha_{s}(\mu)\right)=\sum_{i}\left(\alpha_{s}(\mu)\right)^{i} P_{j k}^{(i)}(z) . \tag{5.2}
\end{equation*}
$$

Coefficient functions and splitting functions are known up to NNLO accuracy [4, 718, 5]. It has been found that at this order large corrections appear which are enhanced by the logarithmic terms in $1 / x$. The collinear approach suffers also from other limitations. The kinematical approximations mostly suitable for the evaluation of the inclusive observables are not sufficient for exclusive processes and can lead to large discrepancies [719].

There are also other direct indications of the breakdown of the fixed order approach. From the global fits [22, 43], it is known that the gluon density suffers from large uncertainties at the NLO level in the region of small values of $x$, and the gluon density even turns negative. Even though the gluon density is not a directly observable quantity, the aforementioned uncertainties propagate into the observable longitudinal structure function $F_{L}$. The problem is concentrated in the low $Q$ and low- $x$ region, though the uncertainties remain even at larger values of $Q$ when $x$ is decreased. A systematic study of the compatibility of the HERA deep inelastic data with DGLAP evolution has been performed in [720]. This analysis, originally based on the NNPDF1.2 analysis [681, 721], was then extended to the global NNPDF2.0 set, which includes the very precise combined HERA-I dataset as well as all the relevant hadronic data. A 'safe' region was defined as the one in which the non-DGLAP effects are expected to be negligible, and it was defined by the cut on low- $x$ and $Q$ data. A fit was then performed to the data that pass the cut and only belong to the safe region and the structure functions evaluated at different scales. It turned out that the prediction for the structure functions at low $Q^{2}$ obtained from the backward-evolution of the data above the cut exhibits a systematic downward trend. Thus the precise HERA measurements indicate that the fixed order DGLAP evolution is incompatible with the data in the low $Q^{2}$ and low $x$ region.

## Small- $x$ re-summations

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Since the seminal works [59, 60], it is well known that observables at small $x$ receive substantial corrections due to the large logarithms $\alpha_{s} \ln 1 / x$ which need to be re-summed in this regime. The BFKL approach [59, 60] provides a framework for this summation and it is known up to next-to-leading logarithmic accuracy. The resulting evolution of the gluon Green's function provided by this framework is with respect to the $\ln 1 / x$ or rapidity variable, with the transverse momenta of the gluons being summed over all possible configurations. The evolution has the following form

$$
\begin{equation*}
G\left(Y ; \mathbf{k}, \mathbf{k}_{0}\right)=\delta^{(2)}\left(\mathbf{k}-\mathbf{k}_{0}\right)+\int d^{2} \mathbf{k}^{\prime} K\left(\mathbf{k}, \mathbf{k}^{\prime}\right) G\left(Y ; \mathbf{k}^{\prime}, \mathbf{k}_{0}\right), \tag{5.3}
\end{equation*}
$$

with the branching kernel having also the perturbative expansion

$$
\begin{equation*}
K\left(\mathbf{k}, \mathbf{k}^{\prime}\right)=\sum_{i}\left(\alpha_{s}(\mu)\right)^{i} K^{(i)}\left(\mathbf{k}, \mathbf{k}^{\prime}\right) . \tag{5.4}
\end{equation*}
$$

A solution for the gluon Green's function and therefore the resulting cross sections exhibit strong growth with the energy, the hard Pomeron, with the intercept being significantly larger than unity in the LO approximation, $\omega_{P}=1+\alpha_{s} N_{c} 4 \ln 2 / \pi$. This growth turns out to be incompatible with both the hadronic data and the data on structure functions from deep-inelastic scattering. NLL (next-to-leading-log) corrections [722, 723] turned out to be rather large numerically and point to the need for the resummation of subsequent powers of higher order corrections $\alpha_{s}^{k} \ln 1 / x$. The sizes of the various NLL corrections can be understood on physical grounds. Firstly, unlike in the DGLAP limit, the strong coupling constant is not naturally a small parameter. On top of that, the BFKL approach does not satisfy the momentum sum rule for the longi-


Figure 5.3. The intercept of the hard Pomeron extracted from the BFKL equation with fixed strong coupling in LL, NLL and re-summed cases. tudinal momentum fractions (the transverse momenta are however conserved, unlike in the collinear approach). The kinematical approximations made in the BFKL limit cannot be efficiently recovered by the truncated higher orders of the perturbative expansion.

The strategy of re-summation at small $x$ has been developed in a series of works [724, 725, 726, 727, 728. It involves the construction of the appropriate re-summed kernel of the form given by Eq. 5.4, which includes at the same time known terms in the expansion of the splitting function, Eq. 5.2. Although the details of the various approaches differ, there are common fundamental ingredients. The evolution in rapidity is subjected to kinematical constraints which originate from the requirement of the consistency of the


Figure 5.4. Left: The gluon Green's function extracted from the BFKL equation in LL and resummed cases. The coupling is running in all computations, and $\bar{k}$ denotes the scale at which the strong coupling is regularized. Right: The extracted effective splitting function from the re-summed approach: solid line. The scale was taken to be $Q=4.5 \mathrm{GeV}$. Dotted pink line indicates the LO DGLAP splitting function and the blue dashed indicates small $x$ part of the NNLO DGLAP. The dashed green line corresponds to the re-summed spliitting function from the $\omega$ expansion. The band correspond to the scale variation.
assumption about the Regge kinematics. The evolution is matched with the DGLAP evolution by including the splitting function at LO and NLO. The momentum sum rule is imposed onto the resulting re-summed splitting function. The running of the coupling is included into the evolution. Finally, matching to the NLL BFKL is performed with the suitable subtractions in order to avoid double counting. The resulting Green's function and splitting function turn out to be very stable with minimal variations across the different re-summation schemes.
c Gluon Green's function and the splitting function: In Fig. 5.3, we show the results on the intercept of the gluon Green's function in the case of the fixed strong coupling constant, obtained within the re-summation framework of [724]. The linear growth is given by the LO approximation. The NLO value of the intercept is significantly below the lowest order, and turns negative even for the intermediate values of $\alpha_{s}$. The re-summed result is between the NLO and LO, it exhibits clear growth with increasing values of the coupling constant, albeit much reduced with respect to the LO value and much closer to the phenomenology.

The rapidity dependence of the gluon Green's function is shown in Fig. 5.4 (left). The scale was chosen to be equal to $k=4.5 \mathrm{GeV}$. The reduction of the speed of growth is clear in the re-summed case. Also the scale variations are relatively small in this case.

By using the deconvolution of the integral equation, one can calculate the integrated gluon density. As a result, it is possible to solve the re-summed splitting function numerically. In this way, the perturbative and non-perturbative contributions are factorized in $Q^{2}$. In Fig. 5.4 (right), we show the results for the splitting function as a function of the momentum fraction for the re-summed case. It is compared with the results on the LO and NNLO (only small $x$ part) splitting functions. The results on the splitting function demonstrate that the small x growth is delayed to much smaller values of x (beyond HERA). The splitting function also has an interesting feature, namely that of the dip. It turns out that
this is a universal feature, present also in other schemes of re-summation. In general, it was found that the dip comes from the interplay between NNLO order and the re-summation.

Thus far, re-summation was demonstrated to give stable results for the gluon channel only. For the complete description, however, one needs to include quarks in the evolution. A matrix approach was developed which was shown to be consistent with the collinear matrix factorization of the parton densities in the singlet evolution 726. This approached enables the calculation of the anomalous dimensions matrix, which can be directly compared with the standard DGLAP matrix. It was shown that it is possible to incorporate NLLx BFKL + NLO DGLAP in this framework [726].

Conclusions and outlook: The small- $x$ regime requires a formalism which incorporates re-summation of the large terms $\alpha_{s} \ln 1 / x$. The BFKL formalism was extended to include re-summation to higher orders. This formalism includes both DGLAP NLO and BFKL NLL and higher order terms. Stability of the results was demonstrated for scale changes and model changes. There are certain universal and characteristic features which come from the solutions to the evolution equations: the rapid growth with $x$ is delayed to smaller values of $x$, and the splitting function has a minimum. A matrix model was developed which gives consistent results on the gluon Green's function and the splitting functions. For the complete framework, one needs to include the re-summed coefficient functions. Detailed fits to the data need to be performed. In this regard, the EIC will generate very important information on parton densities at small $x$, and in distinguishing small $x$ re-summation effects from higher twist saturation effects.

## Parton Saturation

## Yuri V. Kovchegov and Cyrille Marquet

The QCD description of hadrons in terms of quarks and gluons depends on the processes considered and on what part of the hadron wave function they are sensitive to. Consider a hadron moving at nearly the speed of light along the light cone direction $x^{+}$, with momentum $P^{+}$. Depending on their transverse momentum $k_{T}$ and longitudinal momentum $x P^{+}$, the virtual partons inside the hadron behave differently, reflecting the different regimes of the hadron wave function. Soft hadronic processes are mostly sensitive to the non-perturbative part of the wave function, they involve quantum fluctuations with transverse momenta of the order of $\Lambda_{Q C D} \sim 200 \mathrm{MeV}$. A hadron can then be thought of as a bound state of stronglyinteracting partons, but a QCD description of the associated dynamics is still lacking. By contrast, hard processes in hadronic collisions are sensitive to the weakly-coupled part of the wave function and resolve the partonic structure of hadrons. They probe partons with $k_{T} \gg \Lambda_{Q C D}$ whose QCD dynamics is better understood.

One can distinguish two weakly-coupling regimes in the wave function: a linear one called the hard regime, involving a small density of partons, typically with $x \lesssim 1$, in which the hadron looks like a dilute system of independent partons, and a non-linear one called the saturation regime, involving a large density of partons with $x \ll 1$, in which the hadron looks like a dense system of nevertheless weakly-interacting partons, mainly gluons (called small- $x$ gluons). The dilute-dense separation is a bit subtler than that: the larger $k_{T}$ is, the smaller $x$ needs to be to enter the saturation regime. Indeed the separation between the two regimes is characterized by a momentum scale $Q_{s}(x)$, called the saturation scale, which increases as $x$ decreases. In a scattering process, dilute partons (with $k_{T} \gg Q_{s}(x)$ ) behave
incoherently, while when the parton density is large $\left(k_{T} \lesssim Q_{s}(x)\right)$, gluons scatter coherently. The dynamics of the dilute regime is well described by the leading-twist approximation of QCD, whose hallmark is collinear factorization. As explained in the previous section, when $x$ becomes small while not yet reaching the non-linear regime, so-called small- $x$ re-summations are also needed to improve the approximation.

To describe the small- $x$ non-linear part of hadronic/nuclear wave functions in QCD, the Color Glass Condensate (CGC) effective theory was proposed. Rather than using the standard Fock-state expansion which is ineffective in dealing with numerous small-x gluons, the CGC approach employs collective degrees of freedom, static color sources at large $x$ and dynamical classical color fields at small $x$. The traditional approach to saturation physics consists of two stages, corresponding to two different levels of approximations. The first level corresponds to the classical gluon field description of nuclear wave functions and scattering cross sections. It re-sums all multiple re-scatterings in the nucleus, but lacks energy dependence. The latter is included through quantum corrections, which are re-summed by non-linear evolution equations. This constitutes the second level of approximation. We will present both stages below.

## Classical gluon fields

McLerran-Venugopalan model: Imagine a single large nucleus, which was boosted to some ultrarelativistic velocity, as shown in Fig. 5.5(left). We are interested in the dynamics of small- $x$ gluons in the wave function of this relativistic nucleus. The small- $x$ gluons interact with the whole nucleus coherently in the longitudinal direction: therefore, only the transverse plane distribution of nucleons is important for the small- $x$ wave function. As one can see from Fig. [5.5, after the boost, the nucleons, as "seen" by the small- $x$ gluons, appear to overlap with each other in the transverse plane, leading to high parton density. Large occupation numbers of color charges (partons) lead to classical gluon fields dominating the small- $x$ wave function of the nucleus. This is the essence of the McLerran-Venugopalan (MV) model [729, 730, 731]. According to the MV model, the dominant gluon field is given by the solution of the classical Yang-Mills equations $\mathcal{D}_{\mu} F^{\mu \nu}=J^{\nu}$ where the classical color current $J^{\nu}$ is generated by the valence quarks in the nucleons of the nucleus from Fig. 5.5.


Figure 5.5. Left: Large nucleus before and after an ultrarelativistic boost. Right: Unintegrated gluon distribution $\phi\left(x, k_{T}^{2}\right)$ of a large nucleus due to classical gluon fields (solid line). Dashed curve denotes the lowest-order perturbative result.

The Yang-Mills equations were solved for a single nucleus exactly [732, 733] resulting in the unintegrated gluon distribution $\phi\left(x, k_{T}^{2}\right)$ (multiplied by the phase space factor of the gluon's transverse momentum $k_{T}$ ) shown in Fig. 5.5 right as a function of $k_{T}$. (Note that in the MV model, $\phi\left(x, k_{T}^{2}\right)$ is independent of Bjorken-x.) Fig. 5.5 demonstrates the emergence
of the saturation scale $Q_{s}$. As one can see from Fig. 5.5, the majority of gluons in this classical distribution have transverse momentum $k_{T} \approx Q_{s}$. Since in this classical approximation $Q_{s}^{2} \sim A^{1 / 3}$, for a large enough nucleus, all of its small- $x$ gluons would have large transverse momenta $k_{T} \approx Q_{s} \gg \Lambda_{Q C D}$, justifying the applicability of the perturbative approach to the problem. Note that the gluon distribution slows down its growth with decreasing $k_{T}$ for $k_{T}<Q_{s}$ (from power-law of $k_{T}$ to a logarithm) and the distribution saturates.

DIS at high energy: Glauber-Mueller formula: Let us consider deep inelastic scattering (DIS) on a large nucleus. In DIS, the incoming electron emits a virtual photon, which in turn interacts with the proton or nucleus. In the rest frame of the nucleus, the interaction can be thought of as the virtual photon splitting into a quark-antiquark pair, which then interacts with the nucleus (see Fig. 5.6. left panel). Since the light cone lifetime of the $q \bar{q}$ pair is much longer than the size of the target nucleus, the total cross section for the virtual photon-nucleus scattering can be written as a convolution of the virtual photon's light cone wave function (the probability for it to split into a $q \bar{q}$ pair) with the forward scattering amplitude of a $q \bar{q}$ pair interacting with the nucleus

$$
\begin{equation*}
\sigma_{t o t}^{\gamma * A}\left(Q^{2}, x_{B j}\right)=\int \frac{d^{2} x d z}{2 \pi}\left[\Phi_{T}(\underline{x}, z)+\Phi_{L}(\underline{x}, z)\right] d^{2} b N(\underline{x}, \underline{b}, Y) \tag{5.5}
\end{equation*}
$$

with the help of the light-cone perturbation theory [734. Here the incoming photon with virtuality $Q$ splits into a quark-antiquark pair with the transverse separation $\underline{x}$ and the impact parameter (transverse position of the center of mass of the $q \bar{q}$ pair) $\underline{b}$. $Y$ is the rapidity variable given by $Y=\ln \left(s x_{T}^{2}\right) \approx \ln 1 / x_{B j}$. The square of the light cone wave function of $q \bar{q}$ fluctuations of a virtual photon is denoted by $\Phi_{T}(\underline{x}, z)$ and $\Phi_{L}(\underline{x}, z)$ for transverse and longitudinal photons correspondingly, with $z$ being the fraction of the photon's longitudinal momentum carried by the quark. At the lowest order in electromagnetic coupling ( $\alpha_{E M}$ ) $\Phi_{T}(\underline{x}, z)$ and $\Phi_{L}(\underline{x}, z)$ are given by [735, 736]

$$
\begin{gather*}
\Phi_{T}(\underline{x}, z)=\frac{2 N_{c}}{\pi} \sum_{f} \alpha_{E M}^{f}\left\{a_{f}^{2} K_{1}^{2}\left(x_{\perp} a_{f}\right)\left[z^{2}+(1-z)^{2}\right]+m_{f}^{2} K_{0}\left(x_{\perp} a_{f}\right)^{2}\right\},  \tag{5.6}\\
\Phi_{L}(\underline{x}, z)=\frac{2 N_{c}}{\pi} \sum_{f} \alpha_{E M}^{f} 4 Q^{2} z^{2}(1-z)^{2} K_{0}^{2}\left(x_{\perp} a_{f}\right) \tag{5.7}
\end{gather*}
$$

with $a_{f}^{2}=Q^{2} z(1-z)+m_{f}^{2}, x_{\perp}=|\mathbf{x}|$ and $\sum_{f}$ denoting the sum over all relevant quark flavors with quark masses denoted by $m_{f} . \alpha_{E M}^{f}=e_{f}^{2} / 4 \pi$ with $e_{f}$ the electric charge of a quark with flavor $f$.

Our first goal is to calculate the forward scattering amplitude of a quark-anti-quark dipole interacting with the nucleus, which is denoted by $N(\underline{x}, \underline{b}, Y)$ in Eq. (5.5), including all multiple re-scatterings of the dipole on the nucleons in the nucleus.To do this we need to construct a model of the target nucleus. We assume that the nucleons are dilutely distributed in the nucleus [737. There we can represent the dipole-nucleus interaction as a sequence of successive dipole-nucleon interactions, as shown in Fig. 5.6, right panel. Since each nucleon is a color singlet, the lowest order dipole-nucleon interaction in the forward amplitude from Fig. 5.6 is a two-gluon exchange. The exchanged gluon lines in Fig. 5.6 are disconnected at the top: this denotes a summation over all possible connections of these gluon lines either to the quark or to the anti-quark lines in the incoming dipole.


Figure 5.6. Left: Deep inelastic scattering in the rest frame of the target. Right: Deep inelastic scattering in the quasi-classical Glauber-Mueller approximation in $\partial_{\mu} A^{\mu}=0$ gauge.

Re-summation of the diagrams like the one in Fig. 5.6 yields [737]

$$
\begin{equation*}
N(\underline{x}, \underline{b}, Y=0)=1-\exp \left\{-\frac{x_{\perp}^{2} Q_{s}^{2}(\underline{b}) \ln \left(1 / x_{\perp} \Lambda\right)}{4}\right\} \tag{5.8}
\end{equation*}
$$

with the saturation scale defined by

$$
\begin{equation*}
Q_{s}^{2}(\underline{b}) \equiv \frac{4 \pi \alpha_{s}^{2} C_{F}}{N_{c}} \rho T(\underline{b}) \tag{5.9}
\end{equation*}
$$



Figure 5.7. The forward amplitude of the dipolenucleus scattering $N$,plotted as a function of the transverse separation between the quark and the anti-quark in a dipole ( $x_{\perp}$ ) using Eq. (5.8).

Here, $\rho$ is the density of nucleons in the nucleus ( $\rho=A /\left[(4 / 3) \pi R^{3}\right]$ for a spherical nucleus of radius $R$ with atomic number $A$ ) and $T(\underline{b})$ is the nuclear profile function equal to the length of the nuclear medium at a given impact parameter $\underline{b}$, such that $T(\underline{b})=2 \sqrt{R^{2}-\underline{b}^{2}}$ for a spherical nucleus. $\Lambda$ is an infrared cutoff. We put $Y=0$ in the argument of $N$ in Eq. (5.8) to underline that this expression does not include any small- $x$ evolution which would bring in the rapidity dependence.

Eqs. (5.8) and (5.9) allow us to determine the parameter corresponding to the re-summation of the diagrams like the one shown in Fig. 5.6. Noting that for large nuclei, the profile function scales as $T(\underline{b}) \sim$ $A^{1 / 3}$ and the nucleon density scales as $\rho \sim$ $A^{0}$, we conclude that the re-summation parameter of multiple re-scatterings is [738]: $\alpha_{s}^{2} A^{1 / 3}$. The physical meaning of the parameter $\alpha_{s}^{2} A^{1 / 3}$ is rather straightforward: at a given impact parameter the dipole interacts with $\sim A^{1 / 3}$ nucleons exchanging two gluons with each. Since the two-gluon exchange is parametrically of the order $\alpha_{s}^{2}$ we obtain $\alpha_{s}^{2} A^{1 / 3}$ as the re-summation parameter for the quasi-classical approximation.

The dipole amplitude $N$, from Eq. (5.8), is plotted (schematically) in Fig. 5.7 as a function of $x_{\perp}$. One can see that, at small $x_{\perp}, x_{\perp} \ll 1 / Q_{s}$, we have $N \sim x_{\perp}^{2}$ and the amplitude is a rising function of $x_{\perp}$. However, at large dipole sizes $x_{\perp} \gtrsim 1 / Q_{s}$, the growth stops and the amplitude levels off (saturates) at $N=1$. This regime corresponds to the black disk limit for the dipole-nucleus scattering where, for large dipoles, the nucleus appears
as a black disk. To understand that the $N=1$ regime corresponds to the black disk limit, let us note that the total dipole-nucleus scattering cross section is given by:

$$
\begin{equation*}
\sigma_{t o t}^{q \bar{q} A}=2 \int d^{2} b N(\underline{x}, \underline{b}, Y) \tag{5.10}
\end{equation*}
$$

where the integration goes over the cross sectional area of the nucleus. If $N=1$ at all impact parameters $\underline{b}$ inside the nucleus, for a spherical nucleus of radius $R$, Eq. (5.10) becomes $\sigma_{t o t}^{q \bar{q} A}=2 \bar{\pi} R^{2}$, which is a well-known formula for the cross section of a particle scattering on a black sphere [739].

The transition between the $N \sim x_{\perp}^{2}$ to $N=1$ behavior in Fig. 5.7 happens at around $x_{\perp} \sim 1 / Q_{s}$. For dipole sizes $x_{\perp} \gtrsim 1 / Q_{s}$, the amplitude $N$ saturates to a constant. This translates into the saturation of quark distribution functions in the nucleus, as was shown in [737] (as $x q+x \bar{q} \sim F_{2} \sim \sigma_{t o t}^{\gamma * A}$ ), and thus can be identified with parton saturation, justifying the name of the saturation scale.

Before we proceed, let us finally note that since $T(\underline{b}) \sim A^{1 / 3}$, the saturation scale in Eq. (5.9) scales as $Q_{s}^{2} \sim A^{1 / 3}$ with the nuclear atomic number [730, 731, 729, 737]. This implies that for a very large nucleus, the saturation scale would become very large, much larger than $\Lambda_{Q C D}$. If $Q_{s} \gg \Lambda_{Q C D}$, the transition to the black disk limit in Fig. 5.7 happens at momentum scales (corresponding to inverse dipole sizes) where the physics is perturbative and gluons are the correct degrees of freedom.

## Nonlinear evolution equations

General picture: While the classical gluon fields of the MV model exhibit many correct qualitative features of saturation physics, and give predictions about the $A$-dependence of observables which may be compared to the data, they do not lead to any rapidity/Bjorken$x$ dependence of the corresponding observables, which is essential in the data on nuclear and hadronic collisions. To include rapidity dependence, one has to calculate quantum corrections to the classical fields described above.


Figure 5.8. Nonlinear small- $x$ evolution of a hadronic or nuclear wave functions. All partons (quarks and gluons) are denoted by straight solid lines for simplicity.

The inclusion of quantum corrections is accomplished by the small- $x$ evolution equations. The first small- $x$ evolution equation was constructed before the birth of saturation physics. This is the Balitsky-Fadin-Kuraev-Lipatov (BFKL) evolution equation [60, 59]. This is a linear evolution equation, which is illustrated by the first term on the right hand side of Fig. 5.8. Consider a wave function of a high-energy nucleus or hadrons: it contains many partons, as shown on the left of Fig. 5.8. As we make one step of evolution by boosting the nucleus/hadron to higher energy, either one of the partons can split into two partons,
leading to an increase in the number of partons proportional to the number of partons $N$ at the previous step,

$$
\begin{equation*}
\frac{\partial N\left(x, k_{T}^{2}\right)}{\partial \ln (1 / x)}=\alpha_{s} K_{B F K L} \otimes N\left(x, k_{T}^{2}\right) \tag{5.11}
\end{equation*}
$$

with $K_{B F K L}$ an integral kernel. Clearly the BFKL equation (5.11) introduces a Bjorken$x /$ rapidity dependence in the observables it describes.

The main problem with the BFKL evolution is that it leads to the power-law growth of the total cross sections with energy, $\sigma_{t o t} \sim s^{\alpha_{P}-1}$, with the BFKL pomeron intercept $\alpha_{P}-1=\left(4 \alpha_{s} N_{c} \ln 2\right) / \pi>0$. Such a power-law cross section increase violates the Froissart bound, which states that the total hadronic cross section can not grow faster than $\ln ^{2} s$ at very high energies. Moreover, the power-law growth of cross sections with energy violate the black disk limit known from quantum mechanics: the high-energy total scattering cross section $\sigma_{t o t}$ of a particle on a sphere of radius $R$ is bounded by $2 \pi R^{2}$ (note the factor of 2 which is due to quantum mechanics, this is not simply a hard sphere from classical mechanics!).

We see that something has to modify Eq. (5.11) at high energy. The modification is illustrated on the far right of Fig. [5.8: at very high energies, partons may start to recombine with each other on top of the splitting. The recombination of two partons into one is proportional to the number of pairs of partons, which, in turn, scales as $N^{2}$. We end up with the following non-linear evolution equation:

$$
\begin{equation*}
\frac{\partial N\left(x, k_{T}^{2}\right)}{\partial \ln (1 / x)}=\alpha_{s} K_{B F K L} \otimes N\left(x, k_{T}^{2}\right)-\alpha_{s}\left[N\left(x, k_{T}^{2}\right)\right]^{2} . \tag{5.12}
\end{equation*}
$$

This is the Balitsky-Kovchegov (BK) evolution equation [740, 741, which is valid for QCD in the limit of large number of colors $N_{c}$. An equation of this type was originally suggested by Gribov, Levin and Ryskin [742] and by Mueller and Qiu [743, though at the time it was assumed that the quadratic term is only the first non-linear correction with higher order terms possibly appearing as well: in [740, 741 the exact form of the equation was found, and it was shown that in the large- $N_{c}$ limit, Eq. (5.12) does not have any higherorder terms in $N$. Generalization of Eq. (5.12) beyond the large- $N_{c}$ limit is accomplished by the Jalilian-Marian-Iancu-McLerran-Weigert-Leonidov-Kovner (JIMWLK) [744, 745] evolution equation, which is a functional differential equation. Both the BK and JIMWLK evolution equations will be discussed in more details later.

The physical impact of the quadratic term on the right of Eq. (5.12) is clear: it slows down the small- $x$ evolution, leading to parton saturation and to total cross sections adhering to the black disk limit. The effect of gluon mergers becomes important when the quadratic term in Eq. (5.12) becomes comparable to the linear term on the right-hand-side. This gives rise to the saturation scale $Q_{s}$, which now grows with energy (on top of its increase with $A$ ).

The Balitsky-Kovchegov equation: Let us now include the energy dependence in the dipole amplitude $N$ from Eq. (5.8). Similar to the BFKL evolution equation [59, 60, we are interested in quantum evolution in the leading longitudinal logarithmic approximation re-summing the powers of $\alpha_{s} \ln \frac{1}{x_{B j}} \sim \alpha_{s} Y$, with $Y$ the rapidity variable. Again we will be working in the rest frame of the nucleus, but this time we choose to work in the light cone gauge of the projectile $A^{+}=0$ if the dipole is moving in the light cone + direction.

Leading logs in $x$ corrections appear in the diagrams through emissions of long-lived $s$-channel gluons, as shown in Fig. [5.9. These $s$-channel gluons interact with the target


Figure 5.9. Quantum corrections to dipole-nucleus scattering.
nucleus through multiple re-scatterings. In the large- $N_{c}$ limit of QCD such diagrams can be re-summed by the BK evolution equation [740, 746, 741, 747]:

$$
\begin{align*}
\frac{\partial N\left(\underline{x}_{0}, \underline{x}_{1}, Y\right)}{\partial Y}=\frac{\alpha_{s} C_{F}}{\pi^{2}} \int d^{2} x_{2} \frac{x_{01}^{2}}{x_{20}^{2} x_{21}^{2}}\left[N\left(\underline{x}_{0}, \underline{x}_{2}, Y\right)\right. & +N\left(\underline{x}_{2}, \underline{x}_{1}, Y\right)-N\left(\underline{x}_{0}, \underline{x}_{1}, Y\right) \\
& \left.-N\left(\underline{x}_{0}, \underline{x}_{2}, Y\right) N\left(\underline{x}_{2}, \underline{x}_{1}, Y\right)\right] \tag{5.13}
\end{align*}
$$

where we have redefined the arguments of $N$ to depend on the transverse coordinates of the quark and antiquark (instead of dipole size and the impact parameter as was done in Eq. (5.8)). Here $x_{i j}=\left|\underline{x}_{i j}\right|$ and $\underline{x}_{i j}=\underline{x}_{i}-\underline{x}_{j}$.


Figure 5.10. Diagrammatic representation of the nonlinear evolution equation (5.13).
In the large- $N_{c}$ limit, gluon cascades reduce to a cascade of color dipoles. Summation of the dipole cascade is illustrated in Fig. 5.10 where the dipole cascade and its interaction with the target are denoted by a shaded oval. In one step of the evolution in energy (or rapidity) a soft gluon is emitted in the dipole. If the gluon is real, than the original dipole would be split into two dipoles, as shown in Fig. 5.10. Either one of these dipoles can interact with the nucleus with the other one not interacting, which is shown by the first term on the right hand side of Fig. 5.10 with the factor of 2 accounting for the fact that there are two dipoles in the wave function now. Alternatively, both dipoles may interact simultaneously, which is shown by the second term on the right hand side of Fig. 5.10. This term comes in with the minus sign. The emitted gluon in one step of evolution may be a virtual correction, which is not shown in Fig. 5.10: in that case, the original dipole would not split into two, it would remain the same and would interact with the target. In the end, the evolved system of dipoles interacts with the nucleus. In the large- $N_{c}$ limit, each dipole does not interact with other dipoles during the evolution which generates all the dipoles. For a large nucleus, the dipole-nucleus interaction was given above in Eq. (5.8). That result re-sums powers of $\alpha_{s}^{2} A^{1 / 3}$ : hence the BK equation re-sums powers of $\alpha_{s} Y$ and powers of $\alpha_{s}^{2} A^{1 / 3}$.

## Map of high-energy QCD

Solutions of the BK and JIMWLK evolution equations have been calculated numerically [748, 749, 750], with asymptotic limits studied analytically. The numerical solution


Figure 5.11. Left: Solutions of the BK equation at rapidities $\mathrm{Y}=0,5,15$ and 30 (curves are labeled from right to left) for the three different running coupling schemes considered in [751] Right: HERA data on the total DIS $\gamma^{*} p$ cross section plotted in [752] as a function of the scaling variable $\tau=$ $Q^{2} / Q_{s}^{2}\left(x_{B j}\right)$.
(for the BK equation with running coupling, which will be described later) is presented in Fig. 5.11751 . These plots are the same dipole amplitude $N$ plotted as a function of the dipole size labeled $r$ as was done in Fig. 5.7. In Fig. 5.11, different curves correspond to different energies/rapidities $Y$. One can clearly see that the curves tend to drift to the left with increasing energies, corresponding to increasing saturation scale with the energy/rapidity. Therefore we see that the saturation scale increases with rapidity, making the corresponding physics more perturbative.

We summarize our knowledge of high energy QCD in Fig. [5.12, in which different regimes are plotted in the $\left(Q^{2}, Y=\ln 1 / x\right)$ plane, by analogy with DIS. For hadronic and nuclear collisions one can think of typical transverse momentum $p_{T}^{2}$ of the produced particles instead of $Q^{2}$. Also rapidity $Y$ and Bjorken- $x$ variable are interchangeable. On the left of Fig. 5.12 we see the region with $Q^{2} \leq \Lambda_{Q C D}^{2}$ in which the coupling is large, $\alpha_{s} \sim 1$, and small-coupling approaches do not work. In the perturbative region, $Q^{2} \gg \Lambda_{Q C D}^{2}$, we see the standard DGLAP evolution and the linear BFKL evolution. The BFKL equation evolves gluon distributions toward small- $x$, where parton densities becomes large and parton saturation sets in. The transition to saturation is described by the non-linear BK and JIMWLK evolution equations. Most importantly, this transition happens at $Q_{s}^{2} \gg \Lambda_{Q C D}^{2}$ where the small-coupling approach is valid.

One of the most important predictions of nonlinear small-x evolution is that, at high enough rapidity, the scattering amplitude $N$ (and, consequently, DIS structure functions) would be a function of a single variable $x_{\perp} Q_{s}(Y)$, such that $N\left(x_{\perp}, Y\right)=N\left(x_{\perp} Q_{s}(Y)\right)$. This prediction is spectacularly confirmed by HERA data. Geometric scaling has been demonstrated in an analysis of the HERA DIS data [752], presenting one of the strongest arguments for the observation of saturation phenomena at HERA. These results are shown here in Fig. 5.11 from [752], where the authors combined HERA data on the total DIS $\gamma^{*} p$ cross section $\sigma_{\text {tot }}^{\gamma^{*} p}$ for $x_{B j}<0.01$ as a function of the scaling variable $\tau=Q^{2} / Q_{s}^{2}\left(x_{B j}\right)$. One can see that, amazingly enough, all the data falls on the same curve, indicating that $\sigma_{\text {tot }}^{\gamma^{*} p}$ is a function of a single variable $Q^{2} / Q_{s}^{2}\left(x_{B j}\right)$ ! This gives us the best to date experimental proof of geometric scaling. (For a similar analysis of DIS data on nuclear targets see [753].)


Figure 5.12. Map of high energy QCD in the $\left(Q^{2}, Y=\ln 1 / x\right)$ plane.

The fact that geometric scaling is a property of the solution of the BK equation was later demonstrated in 754, 755.

## Universality aspects of the Color Glass Condensate

François Gelis
The Color Glass Condensate (CGC) is an effective field theory (EFT) based on the separation of the degrees of freedom into fast frozen color sources and slow dynamical color fields [729, [731, 730]. A renormalization group equation -the JIMWLK equation [756, 757, 758, 759, 760, 761, 745, 762, 763]- ensures the independence of physical quantities with respect to the cutoff that separates the two kinds of degrees of freedom.

The fast gluons with longitudinal momentum $k^{+}>\Lambda^{+}$are frozen by Lorentz time dilation in configurations specified by a color current $J_{a}^{\mu} \equiv \delta^{\mu+} \rho^{a}$, where $\rho^{a}\left(x^{-}, x_{\perp}\right)$ is the corresponding color charge density. On the other hand, slow gluons with $k^{+}<\Lambda^{+}$are described by the usual gauge fields $A^{\mu}$ of QCD. Because of the hierarchy in $k^{+}$between these two types of degrees of freedom, they are coupled eikonaly by a term $J_{\mu} A^{\mu}$. The fast gluons thus act as sources for the fields that represent the slow gluons. Although it is frozen for the duration of a given collision, the color source density $\rho^{a}$ varies randomly event by event. The CGC provides a gauge invariant distribution $W_{\Lambda^{+}}[\rho]$, which gives the probability of a configuration $\rho$. This encodes all the correlations of the color charge density at the cutoff scale $\Lambda^{+}$, separating the fast and slow degrees of freedom. Given this statistical distribution, the expectation value of an operator at the scale $\Lambda^{+}$is given by

$$
\begin{equation*}
\langle\mathcal{O}\rangle_{\Lambda^{+}} \equiv \int[D \rho] W_{\Lambda^{+}}[\rho] \mathcal{O}[\rho], \tag{5.14}
\end{equation*}
$$

where $\mathcal{O}[\rho]$ is the expectation value of the operator for a particular configuration $\rho$ of the color sources.

The power counting of the CGC EFT is such that in the saturated regime, the sources $\rho$ are of order $g^{-1}$. Attaching an additional source to a given Feynman graph does not alter its order in $g$; the vertex where this new source attaches to the graph is compensated by the
$g^{-1}$ of the source. Thus, computing an observable at a certain order in $g^{2}$ requires the resummation of all the contributions obtained by adding extra sources to the relevant graphs. The leading order in $g^{2}$ is given by a sum of tree diagrams, which can be expressed in terms of classical solutions of the Yang-Mills equations. Moreover, for inclusive observables [764, 765], these classical fields obey a simple boundary condition: they vanish when $t \rightarrow-\infty$.

Next-to-leading order (NLO) computations in the CGC EFT involve a sum of one-loop diagrams embedded in the above classical field. To prevent double counting, momenta in loops are required to be below the cutoff $\Lambda^{+}$. This leads to a logarithmic dependence in $\Lambda^{+}$of these loop corrections. These logarithms are large if $\Lambda^{+}$is well above the typical longitudinal momentum scale of the observable considered, and must be re-summed.

For inclusive observables, the leading logarithms are universal and can be absorbed into a redefinition of the distribution $W_{\Lambda^{+}}[\rho]$ of the hard sources. The evolution of $W_{\Lambda^{+}}[\rho]$ with $\Lambda^{+}$is governed by the functional JIMWLK equation

$$
\begin{equation*}
\frac{\partial W_{\Lambda^{+}}[\rho]}{\partial \ln \left(\Lambda^{+}\right)}=-\mathcal{H}\left[\rho, \frac{\delta}{\delta \rho}\right] W_{\Lambda^{+}}[\rho] \tag{5.15}
\end{equation*}
$$

where $\mathcal{H}$ is known as the JIMWLK Hamiltonian. This operator contains up to two derivatives $\partial / \partial \rho$, and arbitrary powers in $\rho$. Its explicit expression can be found in refs. [756, 757, 758, 759, 760, 761, 745, 762, 763, 766, 767]. The derivation of the JIMWLK equation will be sketched below.

Numerical studies of JIMWLK evolution were performed in [750, 768]. An analytic, albeit formal, solution to the JIMWLK equation was constructed in 769 in the form of a path integral. Alternatively, the evolution can can be expressed as an infinite hierarchy of coupled non-linear equations for $n$-point Wilson line correlators-often called the Balitsky hierarchy [770]. In this framework, the BK equation is a mean field approximation of the JIMWLK evolution, valid in the limit of a large number of colors $N_{c} \rightarrow \infty$. Numerical studies of the JIMWLK equation [750, 768] have found only small differences with the BK equation.

Let us finally comment on the initial condition for the JIMWLK equation which is also important in understanding its derivation. The evolution should start at some cutoff value in the longitudinal momentum scale $\Lambda_{0}^{+}$at which the saturation scale is already a (semi)hard scale, say $Q_{s 0} \gtrsim 1 \mathrm{GeV}$, for perturbation theory to be applicable. The gluon distribution at the starting scale is in general non-perturbative and requires a model. A physically motivated model for the gluon distribution in a large nucleus is the McLerran-Venugopalan model [729, 731, 730]. In a large nucleus, there is a window in rapidity where evolution effects are not large but $x$ is still sufficiently small for a probe not to resolve the longitudinal extent of the nucleus. In this case, the probe "sees" a large number of color charges, proportional to $A^{1 / 3}$. These charges add up to form a higher dimensional representation of the gauge group, and can therefore be treated as classical color distributions [729, 731, 730, 771, Further, the color charge distribution $W_{\Lambda_{0}^{+}}[\rho]$ is a Gaussian distribution ${ }^{11}$ in $\rho$. The variance of this distribution -the color charge squared per unit area- is proportional to $A^{1 / 3}$ and provides a semi-hard scale that makes weak coupling computations feasible. In addition to its role in motivating the EFT and serving as the initial condition in JIMWLK evolution, the MV model allows for direct phenomenological studies in $\mathrm{p}+\mathrm{A}$ and $\mathrm{A}+\mathrm{A}$ collisions in

[^275]regimes where the values of $x$ are not so small as to require evolution.
The CGC in DIS at small $x$ : We denote $\sigma_{\text {dipole }}\left(x, \boldsymbol{r}_{\perp}\right)$ the QCD "dipole" cross-section for the quark-antiquark pair to scatter off the target. This process is shown in fig. 5.13 left, where we have assumed that the target moves in the $-z$ direction. In the leading order (LO) CGC description of DIS, the target is described, as illustrated in fig. 5.13 right, as static sources with $k^{-}>\Lambda_{0}^{-}$. The field modes do not contribute at this order.


Figure 5.13. Left: LO and NLO contributions to DIS off the CGC. Top right: sources and fields in the CGC effective theory. Bottom right: NLO correction from a layer of field modes just below the cutoff.

Employing the optical theorem, $\sigma_{\text {dipole }}\left(x, \boldsymbol{r}_{\perp}\right)$ can be expressed in terms of the forward scattering amplitude $\boldsymbol{T}\left(\boldsymbol{x}_{\perp}, \boldsymbol{y}_{\perp}\right)$ of the $q \bar{q}$ pair at LO as

$$
\begin{equation*}
\sigma_{\text {dipole }}^{\mathrm{LO}}\left(x, \boldsymbol{r}_{\perp}\right)=2 \int d^{2} \mathbf{b} \int[D \rho] W_{\Lambda_{0}^{-}}[\rho] \boldsymbol{T}_{\mathrm{LO}}\left(\boldsymbol{b}+\frac{\boldsymbol{r}_{\perp}}{2}, \boldsymbol{b}-\frac{\boldsymbol{r}_{\perp}}{2}\right), \tag{5.16}
\end{equation*}
$$

where, for a fixed configuration of the target color sources [775, (776]

$$
\begin{equation*}
\boldsymbol{T}_{\mathrm{LO}}\left(\boldsymbol{x}_{\perp}, \boldsymbol{y}_{\perp}\right)=1-\frac{1}{N_{c}} \operatorname{tr}\left(U\left(\boldsymbol{x}_{\perp}\right) U^{\dagger}\left(\boldsymbol{y}_{\perp}\right)\right), \tag{5.17}
\end{equation*}
$$

with $U\left(\boldsymbol{x}_{\perp}\right)$ a Wilson line representing the interaction between a quark and the color fields of the target, defined to be

$$
\begin{equation*}
U\left(\boldsymbol{x}_{\perp}\right)=\mathrm{T} \exp i g \int^{1 / x P^{-}} d z^{+} \mathcal{A}^{-}\left(z^{+}, \boldsymbol{x}_{\perp}\right) . \tag{5.18}
\end{equation*}
$$

In this formula, $\mathcal{A}^{-}$is the minus component of the gauge field generated (in Lorentz gauge) by the sources of the target; it is obtained by solving classical Yang-Mills equations with these sources. The upper bound $x P^{-}$(where $P^{-}$is the target longitudinal momentum) indicates that source modes with $k^{-}<x P^{-}$do not contribute to this scattering amplitude. Thus if the cutoff $\Lambda_{0}^{-}$of the CGC EFT is lower than $x P^{-}, \boldsymbol{T}_{\mathrm{LO}}$ is independent of $\Lambda_{0}^{-}$.

However, when $\Lambda_{0}^{-}$is larger than $x P^{-}$, the dipole cross-section is in fact independent of $x$ (since the CGC EFT does not have source modes near the upper bound $x P^{-}$) and depends on the unphysical parameter $\Lambda_{0}^{-}$. As we shall see now, this is related to the fact that eq. (5.16) is incomplete and receives large corrections from higher order diagrams. Consider now the NLO contributions (one of them is shown in the right panel in figure 5.13 left with gauge field modes in the slice $\Lambda_{1}^{-} \leq k^{-} \leq \Lambda_{0}^{-}$(see fig. 5.13 right). An explicit computation of the contribution of field modes in this slice gives

$$
\begin{equation*}
\delta \boldsymbol{T}_{\mathrm{NLO}}\left(\boldsymbol{x}_{\perp}, \boldsymbol{y}_{\perp}\right)=\ln \left(\frac{\Lambda_{0}^{-}}{\Lambda_{1}^{-}}\right) \mathcal{H} \boldsymbol{T}_{\mathrm{LO}}\left(\boldsymbol{x}_{\perp}, \boldsymbol{y}_{\perp}\right), \tag{5.19}
\end{equation*}
$$

where $\mathcal{H}$ is the JIMWLK Hamiltonian. All dependence on the cutoff scales is in the logarithmic prefactor alone. This Hamiltonian has two derivatives with respect to the classical field $\mathcal{A} \sim \mathcal{O}(1 / g) ; \mathcal{H} \boldsymbol{T}_{\mathrm{LO}}$ is of order $\alpha_{s} \boldsymbol{T}_{\mathrm{LO}}$ and therefore clearly an NLO contribution. However, if the new scale $\Lambda_{1}^{-}$is such that $\alpha_{s} \ln \left(\Lambda_{0}^{-} / \Lambda_{1}^{-}\right) \sim 1$, this NLO term becomes comparable in magnitude to the LO contribution. Averaging the sum of the LO and NLO contributions over the distribution of sources at the scale $\Lambda_{0}^{-}$, one obtains

$$
\begin{equation*}
\int[D \rho] W_{\Lambda_{0}^{-}}[\rho]\left(\boldsymbol{T}_{\mathrm{LO}}+\delta \boldsymbol{T}_{\mathrm{NLO}}\right)=\int[D \rho] W_{\Lambda_{1}^{-}}[\rho] \boldsymbol{T}_{\mathrm{LO}}, \tag{5.20}
\end{equation*}
$$

where $W_{\Lambda_{1}^{-}} \equiv\left(1+\ln \left(\Lambda_{0}^{-} / \Lambda_{1}^{-}\right) \mathcal{H}\right) W_{\Lambda_{0}^{-}}$. We have shown here that the NLO correction from quantum modes in the slice $\Lambda_{1}^{-} \leq k^{-} \leq \Lambda_{0}^{-}$can be absorbed in the LO term, provided we now use a CGC effective theory at $\Lambda_{1}^{-}$with the modified distribution of sources shown in eq. (5.20). In differential form, the evolution equation of the source distribution is the JIMWLK equation stated previously.

Repeating this elementary step, one progressively re-sums quantum fluctuations down to the scale $k^{-} \sim x P^{-}$. Thanks to eq. (5.20), the result of this re-summation for the dipole cross-section is formally identical to eq. (5.16), except that the source distribution is $W_{x P^{-}}$ instead of $W_{\Lambda_{0}^{-}}$. Note that if one further lowers the cutoff below $x P^{-}$, the dipole crosssection remains unchanged.

The CGC in A+A collisions: Collisions between two nuclei ("dense-dense" scattering) are complicated to handle on the surface. However, in the CGC framework, because the wave functions of the two nuclei are saturated, the collision can be treated as the collision of classical fields coupled to fast partons of each nucleus respectively described by the external current $J^{\mu}=\delta^{\mu+} \rho_{1}+\delta^{\mu-} \rho_{2}$. The source densities of fast partons $\rho_{1,2}$ are both parametrically of order $1 / g$, which implies that graphs involving multiple sources from both projectiles must be re-summed.

At leading order, inclusive observables ${ }^{2}$ depends on the retarded classical color field $\mathcal{A}^{\mu}$, which solves the Yang-Mills equations $\left[\mathcal{D}_{\mu}, \mathcal{F}^{\mu \nu}\right]=J^{\nu}$ with the boundary condition $\lim _{x^{0} \rightarrow-\infty} \mathcal{A}^{\mu}=0$. Among the observables to which this result applies is the expectation value of the energy-momentum tensor at early times after the collision. At leading order,

$$
\begin{equation*}
T_{\mathrm{LO}}^{\mu \nu}=\frac{1}{4} g^{\mu \nu} \mathcal{F}^{\lambda \sigma} \mathcal{F}_{\lambda \sigma}-\mathcal{F}^{\mu \lambda} \mathcal{F}_{\lambda}^{\nu}, \tag{5.21}
\end{equation*}
$$

where $\mathcal{F}^{\mu \nu}$ is the field strength of the classical field $\mathcal{A}^{\mu}$.
Although $\mathrm{A}+\mathrm{A}$ collisions are more complicated than $\mathrm{e}+\mathrm{A}$ or $\mathrm{p}+\mathrm{A}$ collisions, one can still factorize the leading higher order corrections into the evolved distributions $W_{\Lambda^{-}}\left[\rho_{1}\right]$ and $W_{\Lambda^{+}}\left[\rho_{2}\right]$. At the heart of this factorization is a generalization of eq. (5.19) to the case where the two projectiles are described in the CGC framework [777, 778, 779]. When one integrates out the field modes in the slices $\Lambda_{1}^{ \pm} \leq k^{ \pm} \leq \Lambda_{0}^{ \pm}$, the correction to the energy momentum tensor is

$$
\begin{equation*}
\delta T_{\mathrm{NLO}}^{\mu \nu}=\left[\ln \left(\frac{\Lambda_{0}^{-}}{\Lambda_{1}^{-}}\right) \mathcal{H}_{1}+\ln \left(\frac{\Lambda_{0}^{+}}{\Lambda_{1}^{+}}\right) \mathcal{H}_{2}\right] T_{\mathrm{LO}}^{\mu \nu} \tag{5.22}
\end{equation*}
$$

where $\mathcal{H}_{1,2}$ are the JIMWLK Hamiltonians of the two nuclei respectively. What is crucial here is the absence of mixing between the coefficients $\mathcal{H}_{1,2}$ of the logarithms of the two

[^276]projectiles; they depend only on $\rho_{1,2}$ respectively and not on the sources of the other projectile. Although the proof of this expression is somewhat involved, the absence of mixing is deeply rooted in causality. The central point is that because the duration of the collision (which scales as the inverse of the energy) is so brief, soft radiation must occur before the two nuclei are in causal contact. Thus logarithms associated with this radiation must have coefficients that do not mix the sources of the two projectiles.

Following the same procedure for eq. (5.22), as for the e+A and p+A cases, one obtains for the energy-momentum tensor in an $\mathrm{A}+\mathrm{A}$ collision the expression

$$
\begin{equation*}
\left\langle T^{\mu \nu}\right\rangle_{\mathrm{LLog}}=\int\left[D \rho_{1} D \rho_{2}\right] W_{1}\left[\rho_{1}\right] W_{2}\left[\rho_{2}\right] T_{\mathrm{LO}}^{\mu \nu} \tag{5.23}
\end{equation*}
$$

This result can be generalized to multi-point correlations of the energy-momentum tensor,

$$
\begin{equation*}
\left\langle T^{\mu_{1} \nu_{1}}\left(x_{1}\right) \cdots T^{\mu_{n} \nu_{n}}\left(x_{n}\right)\right\rangle_{\mathrm{LLog}}=\int\left[D \rho_{1} D \rho_{2}\right] W_{1}\left[\rho_{1}\right] W_{2}\left[\rho_{2}\right] T_{\mathrm{LO}}^{\mu_{1} \nu_{1}}\left(x_{1}\right) \cdots T_{\mathrm{LO}}^{\mu_{n} \nu_{n}}\left(x_{n}\right) . \tag{5.24}
\end{equation*}
$$

In this expression, all the correlations between the energy-momentum tensor at different points are from the distributions $W_{1,2}\left[\rho_{1,2}\right]$. Thus, the leading correlations are already built into the wavefunctions of the projectiles prior to the collision.

Note that the expressions in eqs. (5.23) and (5.24) are valid for proper times $\tau \sim 1 / Q_{s}$ after the heavy ion collision. Complicated final state effects, possibly driven by instabilities, are expected to bring this non-equilibrium gluonic matter into a quark-gluon plasma. Although this aspect of $\mathrm{A}+\mathrm{A}$ collisions is very different from what happens in DIS reactions, the Color Glass Condensate provides a universal description of the hadronic and nuclear wavefunctions prior to the collision in both cases, and a powerful framework to show that the logarithms of the collision energy are universal for inclusive enough observables. Thanks to this universality, measurements at small $x$ in $\mathrm{e}+\mathrm{A}$ collisions can provide valuable constraints on the distributions $W[\rho]$ for a nucleus, that can then be used in order to compute the state of the system formed at early times in A+A collisions.

## Shadowing

## Boris Z. Kopeliovich

In terms of the dipole formalism, nuclear shadowing is related to the interaction of different Fock components of the projectile particle with the nuclear target. The lowest Fock states (i.e. $\gamma^{*} \rightarrow \bar{q} q$ ) are responsible for higher twist shadowing, while higher Fock components (i.e. $\gamma^{*} \rightarrow \bar{q} q g$ ) give rise to leading twist gluon shadowing.

Quark shadowing: The magnitude of higher twist shadowing is controlled by the interplay between two fundamental quantities.
(i) The lifetime of photon fluctuations, or coherence time.

$$
\begin{equation*}
l_{c}=\frac{2 \nu}{Q^{2}+M^{2}}=\frac{P}{x_{B j} m_{N}}=P l_{c}^{\max }, \tag{5.25}
\end{equation*}
$$

where $x_{B j}=Q^{2} / 2 m_{N} \nu, M$ is the effective mass of the fluctuation, $P=\left(1+M^{2} / Q^{2}\right)^{-1}$, and $l_{c}^{\max }=1 / m_{N} x_{B j}$. The usual approximation is to assume that $M^{2} \approx Q^{2}$ since $Q^{2}$ is the only large dimensional scale available. In this case, $P=1 / 2$ and the corresponding value of $l_{c}$ is called Ioffe length of time.

Shadowing is possible only if the coherence time exceeds the mean nucleon spacing in nuclei, and shadowing saturates (for a given Fock component) if the coherence time substantially exceeds the nuclear radius.
(ii) Equally important for shadowing is the transverse separation of the $\bar{q} q$. This controls the dipole-nucleon cross section $\sigma_{\bar{q} q}^{N}(r)$, and correspondingly the total nuclear cross section 780, 781,

$$
\begin{equation*}
\left(\sigma_{\text {tot }}^{\gamma^{*} A}\right)_{l c \gg R_{A}}^{T, L}=2 \int d \alpha \int d^{2} r\left|\Psi_{\bar{q} q}^{T, L}(\varepsilon r)\right|^{2} \int d^{2} b\left[1-\exp \left(-\frac{1}{2} \sigma_{q \bar{q}}^{N}(r) T_{A}(b)\right)\right] \tag{5.26}
\end{equation*}
$$

where the perturbative light-cone distribution function for the $\bar{q} q$ has the form [782, 783],

$$
\begin{equation*}
\Psi_{\bar{q} q}^{T, L}\left(\vec{r}_{T}, \alpha\right)=\frac{\sqrt{\alpha_{e m}}}{2 \pi} \bar{\chi} \widehat{O}^{T, L} \chi K_{0}\left(\epsilon r_{T}\right) ; \tag{5.27}
\end{equation*}
$$

$\chi$ and $\bar{\chi}$ are the spinors of the quark and antiquark respectively; $K_{0}\left(\epsilon r_{T}\right)$ is the modified Bessel function; $\epsilon^{2}=\alpha(1-\alpha) Q^{2}+m_{q}^{2}$; and the operators $\widehat{O}^{T, L}$ for transversely and longitudinally polarized photons have the form,

$$
\begin{gather*}
\widehat{O}^{T}=m_{q} \vec{\sigma} \cdot \vec{e}+i(1-2 \alpha)(\vec{\sigma} \cdot \vec{n})\left(\vec{e} \cdot \vec{\nabla}_{r}\right)+(\vec{\sigma} \times \vec{e}) \cdot \vec{\nabla}_{r},  \tag{5.28}\\
\widehat{O}^{L}=2 Q \alpha(1-\alpha) \vec{\sigma} \cdot \vec{n} . \tag{5.29}
\end{gather*}
$$

Here $\vec{n}=\vec{p} / p$ is a unit vector parallel to the photon momentum; $\vec{e}$ is the polarization vector of the photon; $m_{q}$ and and $\alpha$ are the mass, and fractional light-cone momentum carried by the quark. See also eqs. (5.6) and (5.7) discussed previously.

In order to be shadowed, a $\bar{q} q$-fluctuation of the photon has to interact with a large cross section. As a result of color transparency [780, [784], small size dipoles with $r^{2} \sim$ $1 / Q^{2}$ interact only weakly and are therefore less shadowed. The dominant contribution to shadowing comes from the aligned jet configurations $(\alpha \rightarrow 0,1)$ [785] of $\bar{q} q$ pairs, which have large transverse separation, $\left\langle r^{2}\right\rangle \sim 1 /\left[Q^{2} \alpha(1-\alpha)\right]$ according to (5.27). Although the weight of such configurations is small, $1 / Q^{2}$, this is compensated by the large interaction cross section [786].

The coherence length (Eq. (5.25)) averaged over interacting $|\bar{q} q\rangle$ and $|\bar{q} q g\rangle$ fluctuations calculated in [787] is presented in Fig. 5.14. The mean values of the factor $P=l_{c} / l_{c}^{\max }$ in (5.25) are plotted for $\bar{q} q$ fluctuations of transverse and longitudinal photons, as well as for $\bar{q} q g$ fluctuations as a function of $Q^{2}$ at fixed $x_{B j}$ (left panel). We see that $\bar{q} q$ fluctuations in a longitudinal photon live about twice as long as in a transverse one. Both are different from $P=1 / 2$ corresponding to the Ioffe time. The lifetime of the higher order Fock states containing gluons is about order of magnitude shorter.

Onset of shadowing: Eq. (5.26) describing quark shadowing is valid only in the limit of $l_{c} \gg R_{A}$, i.e. at very small $x_{B j}$ where the magnitude of shadowing nearly saturates. However, all available data for DIS on nuclei are in the region of shorter coherence length, and one needs theoretical tools to describe the onset of shadowing.

The Gribov theory of inelastic shadowing [791] relates nuclear shadowing to the cross section of diffractive dissociation. In the case of a deuteron target, this approach provides a full and model independent description of shadowing. The onset of shadowing can be accurately calculated, since the phase shift $\Delta z / l_{c}$ between the impulse approximation term and the inelastic shadowing term is under control. However, a description of shadowing



Figure 5.14. Left panel: Factor $\left\langle P^{T, L}\right\rangle$ and $\left\langle P^{g}\right\rangle$ defined in (5.25) for $\bar{q} q$ fluctuations of transverse and longitudinal photons, and for $\bar{q} q g$ fluctuations, from the top to bottom. Calculations are done as a function of $Q^{2}$ at $x_{B j}=0.01$. Dotted curves correspond to perturbative wave functions and an approximate dipole cross section $\propto r_{T}^{2}$. Dashed curves rely on the realistic parameterization for the dipole cross section [788]. The solid curves show the most realistic case based on the nonperturbative wave functions. Right panel: Comparison between calculations for quark shadowing and experimental data from NMC [789, 790] for the structure functions of different nuclei relative to carbon as function of $x_{B j}$. The $Q^{2}$ range covered by the data is approximately $3 \mathrm{GeV}^{2} \leq Q^{2} \leq 17 \mathrm{GeV}^{2}$ from the lowest to the highest $x_{B j}$ bin. Solid and dashed curves are calculated with and without the real part of the light-cone potential in (5.31).
for heavy nuclei is a challenge in this approach. Indeed, only the lowest order of Gribov corrections can be calculated using data on diffraction. The higher order corrections, illustrated in Fig. 5.15a, need information unavailable from data, like the diffractive amplitudes between different excited states, $X^{*}, X^{* *}$, the attenuation of these states in the nuclear medium, etc.

a

b

Figure 5.15. a: A high order term in Gribov inelastic shadowing corrections to $F_{2}^{A}\left(x, Q^{2}\right)$; b: Dipole description based on the path integral technique, which sums up the Gribov corrections in all orders.

An alternative description with the path integral technique was proposed in [787. One should sum up over all possible trajectories of the quark and antiquark propagating through the nucleus, as is illustrated in Fig. 5.15 b. This leads to the 2-dimensional Schrödinger equation for the Green function describing propagation of a dipole with initial (final) transverse
separation $\vec{r}_{1}\left(\vec{r}_{2}\right)$ at longitudinal coordinate $z_{1}\left(z_{2}\right)$,

$$
\begin{equation*}
\left[i \frac{\partial}{\partial z_{2}}+\frac{\Delta_{\perp}\left(r_{2}\right)-\varepsilon^{2}}{2 \nu \alpha(1-\alpha)}+\frac{i}{2} \rho_{A}\left(b, z_{2}\right) \sigma_{q \bar{q}}^{N}\left(r_{2}\right)-\frac{a^{4}(\alpha) r_{2}^{2}}{2 \nu \alpha(1-\alpha)}\right] G\left(r_{2}, z_{2} \mid r_{1}, z_{1}\right)=0 \tag{5.30}
\end{equation*}
$$

The last two terms represent the imaginary and real parts of the light cone potential. The former describes the attenuation of the dipole in the nuclear medium, while the latter models the non-perturbative interactions inside the dipole. Solving this equation, one can calculate the shadowing corrections as

$$
\begin{align*}
& \left(\sigma_{\text {tot }}^{\gamma^{*} A}\right)^{T, L}=A\left(\sigma_{\text {tot }}^{\gamma^{*} N}\right)^{T, L}-\frac{1}{2} R e \int d^{2} b \int_{0}^{1} d \alpha \int_{-\infty}^{\infty} d z_{1} \int_{z_{1}}^{\infty} d z_{2} \int d^{2} r_{1} \int d^{2} r_{2}  \tag{5.31}\\
\times & {\left[\Psi_{\bar{q} q}^{T, L}\left(\varepsilon, \lambda, r_{2}\right)\right]^{*} \rho_{A}\left(b, z_{2}\right) \sigma_{q \bar{q}}^{N}\left(s, r_{2}\right) G\left(r_{2}, z_{2} \mid r_{1}, z_{1}\right) \rho_{A}\left(b, z_{1}\right) \sigma_{q \bar{q}}^{N}\left(s, r_{1}\right) \Psi_{\bar{q} q}^{T, L}\left(\varepsilon, \lambda, r_{1}\right) }
\end{align*}
$$

At $l_{c} \ll 1 / \rho \sigma$, the second term vanishes. For $l_{c} \gg R_{A}$, it saturates at the value given by Eq. (5.26). The numerical results are compared with data from the NMC experiment [789, 790] in the right panel of Fig. 5.14. The solid and dashed curves are calculated with and without the real part of the light-cone potential in (5.31). It worth emphasizing that this is a parameter-free calculation, no adjustment to nuclear data has been done. The dipole cross section was fitted to DIS data on a proton.

Note that these calculations were performed for the lowest Fock component $|\bar{q} q\rangle$ of the photon; they miss gluon shadowing related to the higher Fock states containing gluons.

Gluon shadowing: Gluon shadowing is related to specific channels of diffractive gluon radiation. In terms of Regge phenomenology, these processes correspond to the triplePomeron contribution, and can be seen in data as the large mass tail of the invariant mass distribution, $d \sigma_{d i f f} / d M_{X}^{2} \propto 1 / M_{X}^{2}$. Such an $M_{X}^{2}$-dependence is the undebatable evidence of radiation of a vector particle, i.e. a gluon.

Data show that the magnitude of diffractive gluon radiation is amazingly small. The way to see that is to express the single diffraction cross section in terms of the Pomeronproton cross section as is illustrated in the left panel of Fig. 5.16. The Pomeron can be



Figure 5.16. Left panel: The amplitude squared of diffractive excitation of the projectile proton, summed over all the excitations with invariant mass $M_{X}$, is related via the optical theorem with the total Pomeron-proton cross section at c.m. energy $M_{X}$. Right panel: The Pomeron-proton cross section extracted 792 from data on single diffraction $p p \rightarrow p X$ as function of $\mathbb{P}-p$ c.m. squared.
treated as a gluonic dipole and its cross section is expected to be about twice as big as for a $\bar{q} q$ dipole, i.e. $\sigma_{t o t}^{\mathbb{P P} p} \sim 50 \mathrm{mb}$. However, data depicted in the right panel of Fig. 5.16 show
that $\sigma_{\text {tot }}^{\mathbb{P p}}<2 \mathrm{mb}$. Such a dramatic disagreement gives a clue that diffractive gluon radiation is strongly suppressed compared with the expectation based on pQCD . This problem has been known in the Regge phenomenology as smallness of the triple-Pomeron coupling [793].

Gluon radiation can be described within the dipole approach via the propagation of a $\bar{q} q g$ dipole through the nuclear medium [794]. As the mean fractional momentum of the radiated gluon is very small, $\left\langle\alpha_{g}\right\rangle \sim 1 / \ln (s)$, one can rely on eq. (5.26) for very small $x_{B j}$, or eqs. (5.30)-(5.31) for the onset of gluon shadowing, by replacing $\sigma_{\bar{q} q}(r) \Rightarrow \sigma_{g g}(r)$. The only way to explain the observed suppression of gluon radiation is to reduce the mean size of the glue-glue dipole. This can be achieved by introducing a specifically strong nonperturbative interaction within the glue-glue dipole, which comes as the real part of the light-cone potential in eq. (5.30). Adjusting the strength of this interaction to data on diffractive gluon radiation (triple-Pomeron term) one arrives at the light-cone distribution functions in (5.26) and (5.31) with the mean glue-glue separation $r_{0} \approx 0.3 \mathrm{fm}$ [795]. This distance is smaller than the confinement radius $\sim 1 / \Lambda_{Q C D}=1 \mathrm{fm}$ and is in accord with the lattice evaluations of the $g g$ correlation radius [796], and the instanton radius [797]. There is more experimental evidence supporting the existence of a semi-hard scale in hadrons [798].

Thus, the magnitude of gluon shadowing evaluated in [795, 799] is expected to be rather small, as is depicted in Fig. 5.17. The nuclear ratio $R_{g}=G_{A}\left(x, Q^{2}\right) / A G_{N}\left(x, Q^{2}\right)$ is plotted as a function of $x_{B j}$ at $Q^{2}=4$ and $40 \mathrm{GeV}^{2}$ (left panel); and as a function of the path length in nuclear matter at $Q^{2}=4 \mathrm{GeV}^{2}$ and different values of $x_{B j}$.


Figure 5.17. Left panel: Ratio of the gluon distribution functions in nuclei (carbon, copper and lead) and nucleons versus Bjorken $x$ at $Q^{2}=4 \mathrm{GeV}^{2}$ (solid curves) and $40 \mathrm{GeV}^{2}$ (dashed curves) [795). Right panel: Nuclear ratio $R_{g}=G_{A}\left(x, Q^{2}\right) / A G_{N}\left(x, Q^{2}\right)$ for gluons as function of path length in nuclear matter, calculated in 799 at $Q^{2}=4 \mathrm{GeV}^{2}$ for several fixed values of $x$.

The path-integral approach is the most accurate method, which is valid in all regimes of gluon radiation, from incoherent to fully coherent. Nevertheless, this is still the lowest order calculation, which might be a reasonable approximation only for light nuclei, or for the onset of shadowing. The contribution of higher Fock components is still a challenge. This problem has been solved so far only in the unrealistic limit of long coherence lengths for all radiated gluons, described by the Balitsky-Kovchegov (BK) equation [740, 741. A numerical solution of this equation is quite complicated and includes lots of modelling [800]. A much simpler bootstrap equation, which only requires modelling the shape of the saturated gluon distribution, was derived in [801. It includes the self-quenching effect for gluon shadowing, and leads to a gluon distribution in nuclei which satisfies the unitarity bound 802 The results are quite similar to the numerical solutions of the BK equation 800. The magnitude of the self-quenched gluon shadowing found in 801 is similar to the above results obtained in the leading order.

## Leading-twist nuclear shadowing

## Vadim Guzey and Mark Strikman

Nuclear shadowing in hadron (photon)-nucleus scattering is the firmly established experimental phenomenon that at high energies the scattering cross section on a nuclear target is smaller than the sum of the scattering cross sections on the individual nucleons. In the nucleus rest frame, the theory of nuclear shadowing is based on the connection between nuclear shadowing and diffraction which has been established long time ago by Gribov [791]. In the derivation, the key assumption is that nuclei can be described as dilute systems of nucleons. The accuracy of the resulting theory for hadron-nucleus cross sections is very high, with the corrections at the level of a few $\%$ which reflect the small admixture of nonnucleonic degrees of freedom in nuclei and the small off-shellness of the nucleons in nuclei as compared to the soft strong interaction scale. Gribov's result can be understood 803] as a manifestation of unitarity as reflected in the Abramovsky-Gribov-Kancheli (AGK) cutting rules 804 .

The connection between shadowing and diffraction is also valid in deep inelastic scattering (DIS) with nuclei; the approach based on this connection is called the leading twist theory of nuclear shadowing [803, 805, 806, 807. In this theory, parton distribution functions (PDFs) in nuclei at small $x$ are calculated combining the unitarity relations for different cuts of the shadowing diagrams corresponding to the diffractive and inelastic final states (AGK cutting rules) with the QCD factorization theorem for hard diffraction 808 (which provides a good description of the totality of the HERA hard diffractive data). The resulting multiple scattering series for the quark nuclear PDFs is presented in fig. 5.18, where graphs $a, b$, and $c$ correspond to the interaction with one, two, and three nucleons of the target, respectively. Graph $a$ gives the impulse approximation; graphs $b$ and $c$ contribute to the shadowing correction. The interaction with $N>3$ nucleons, though not shown, is taken into account in the final expression for nuclear PDFs.

At the level of the interaction with two nucleons of a nucleus with the atomic mass number $A$, one can derive the model-independent expression for the shadowing correction to the nuclear PDF of flavor $j$ [803] (corresponding to graph $b$ of fig. [5.18):

$$
\begin{align*}
x f_{j / A}^{(b)}\left(x, Q^{2}\right) & =-8 \pi A(A-1) \Re e \frac{(1-i \eta)^{2}}{1+\eta^{2}} \int_{x}^{0.1} d x_{\mathbb{P}} \beta f_{j}^{D(4)}\left(\beta, Q^{2}, x_{\mathbb{P}}, t_{\min }\right) \\
& \times \int d^{2} \vec{b} \int_{-\infty}^{\infty} d z_{1} \int_{z_{1}}^{\infty} d z_{2} \rho_{A}\left(\vec{b}, z_{1}\right) \rho_{A}\left(\vec{b}, z_{2}\right) e^{i\left(z_{1}-z_{2}\right) x_{\mathbb{P}} m_{N}}, \tag{5.32}
\end{align*}
$$

where $f_{j}^{D(4)}$ is the diffractive parton distribution of the nucleon; $\rho_{A}$ is the nuclear matter density; $\eta$ is the ratio of the real to imaginary parts of the elementary diffractive amplitude, $\eta=\Re e A^{\text {diff }} / \Im m A^{\text {diff }} \approx 0.17$. The diffractive $\operatorname{PDF} f_{j}^{D(4)}$ depends on two light-cone fractions $x_{\mathbb{P}}=\left(M_{X}^{2}+Q^{2}\right) /\left(W^{2}+Q^{2}\right)$ and $\beta=x / x_{\mathbb{P}}$ and the invariant momentum transfer $t$, where $W$ is the invariant virtual photon-nucleon energy, $W^{2}=(q+p)^{2}$, and $M_{X}^{2}$ is the invariant mass squared of the produced intermediate diffractive state denoted as "X" in fig. 5.18. The longitudinal (collinear with the direction of the photon momentum) coordinates $z_{1}$ and $z_{2}$ and the transverse coordinate (impact parameter) $\vec{b}$ refer to the two interacting nucleons; $m_{N}$ is the nucleon mass. The $t$ dependence of $f_{j}^{D(4)}$ can be safely neglected as compared to the strong fall-off of the nuclear form-factor for $A>4$ and, as a result, $f_{j}^{D(4)}$ enters eq. (5.32) at $t_{\min } \approx-x^{2} m_{N}^{2}\left(1+M_{X}^{2} / Q^{2}\right)^{2}$ and all nucleons enter with the same impact


Figure 5.18. Multiple scattering series for nuclear quark PDFs. Graphs $a, b$, and $c$ correspond to the interaction with one, two, and three nucleons, respectively. Graph $a$ gives the impulse approximation; graphs $b$ and $c$ contribute to the shadowing correction.
parameter $\vec{b}$. Equation (5.32) satisfies the QCD evolution equations at all orders in the strong coupling constant $\alpha_{s}$.

To evaluate the contribution to nuclear shadowing of the interactions with $N \geq 3$ nucleons in fig. 5.18, one needs to invoke additional model-dependent considerations, since the interaction of a hard probe (virtual photon) with $N \geq 3$ nucleons is sensitive to fine details of the diffractive dynamics. In particular, the hard probe can be viewed as a coherent superposition of configurations which interact with the target nucleons with very different strengths. This effect of color (cross section) fluctuations is analogous to the inelastic shadowing in hadron-nucleus scattering with the important difference that the dispersion of the interaction strengths is much smaller in the hadron case than in DIS. However, the observation that $\alpha_{\mathbb{P}}(0)=1.11$ found in the analysis of hard diffraction at HERA [809] is very close to $\alpha_{P}^{\text {soft }}(0)=1.08$ in soft hadronic interactions [810] indicates that hard diffraction in DIS is dominated by large-size hadron-like (aligned jet) configurations which evolve to large $Q^{2}$ via the DGLAP evolution. (As to the point-like configurations, they give an important and increasing with $Q^{2}$ contribution to graph $a$ in fig. 5.18.)

This important observation reduces theoretical uncertainties in the treatment of the interactions with $N \geq 3$ nucleons and allows one to reliably parameterize the strength of the interaction with $N \geq 3$ nucleons by a single effective hadron-like cross section $\sigma_{\text {soft }}^{j}$. The final expression for the nuclear PDFs at a certain initial scale $Q_{0}^{2}$ reads [806, 807]:

$$
\begin{align*}
x f_{j / A}\left(x, Q_{0}^{2}\right) & =A x f_{j / N}\left(x, Q_{0}^{2}\right) \\
& -8 \pi A(A-1) \Re e \frac{(1-i \eta)^{2}}{1+\eta^{2}} \int_{x}^{0.1} d x_{\mathbb{P}} \beta f_{j}^{D(4)}\left(\beta, Q_{0}^{2}, x_{\mathbb{P}}, t_{\min }\right) \int d^{2} b \int_{-\infty}^{\infty} d z_{1} \\
& \int_{z_{1}}^{\infty} d z_{2} \rho_{A}\left(\vec{b}, z_{1}\right) \rho_{A}\left(\vec{b}, z_{2}\right) e^{i\left(z_{1}-z_{2}\right) x_{\mathbb{P}} m_{N}} e^{-\frac{A}{2}(1-i \eta) \sigma_{\text {soft }}^{j}\left(x, Q_{0}^{2}\right) \int_{z_{1}}^{z_{2}} d z^{\prime} \rho_{A}\left(\vec{b}, z^{\prime}\right)} . \tag{5.33}
\end{align*}
$$

Due to the QCD factorization theorem, these nuclear PDFs $f_{j / A}\left(x, Q^{2}\right)$ can be used to calculate many different observables at small $x$ including the nuclear structure function $F_{2 A}$ and the longitudinal structure function $F_{L}^{A}$, the charmed contributions to these structure functions $F_{2 A}^{c}$ and $F_{L}^{A(c)}$, etc.; $f_{j / A}\left(x, Q^{2}\right)$ can also be applied to the calculations of hard processes in heavy-ion collisions.

Removing the integration over $d^{2} b$ in right-hand side of eq. (5.33), one obtains the impact parameter dependent nuclear PDFs (nuclear GPDs in the $\xi=0$ limit in the impact parameter representation) 807, see Section 5.9.1.


Figure 5.19. The leading twist theory of nuclear shadowing predictions for $f_{j / A} /\left(A f_{j / N}\right)$ ( $\bar{u}$ and $c$ quarks and gluons) and $F_{2 A} /\left(A F_{2 N}\right)$ as functions of $x$ at $Q_{0}^{2}=4 \mathrm{GeV}^{2}$. The two sets of curves correspond to the two extreme scenarios of nuclear shadowing (see the text).

In our analysis 807, we used two models for the color fluctuations in the virtual photon which correspond to two models for $\sigma_{\text {soft }}^{j}$ which cover essentially all reasonable possibilities for the resulting nuclear shadowing. An example of our predictions for the gluon, $\bar{u}$ quark, $c$-quarks, and $F_{2 A}$ structure functions is presented in fig. 5.19 for the two scenarios for $\sigma_{\text {soft }}^{j}$ that we have mentioned above (labeled FGS10_H and FGS10_L). As one can see from fig. 5.19, we predict large nuclear shadowing for each singlet parton flavor with the characteristic feature that nuclear shadowing in the gluon channel is larger than that in the quark channel. The difference between the two extreme scenarios of color fluctuations (the solid and dotted curves in fig. 5.19) is less than $20 \%$ for $A \sim 200$ and much smaller for light nuclei. The spread between the solid and dotted curves is the theoretical uncertainty of our predictions. Note also that these results weakly depend on the choice of nucleon PDFs.

Accounting for the color fluctuations as done in eq. (5.33) tends to reduce the amount of nuclear shadowing as compared to the quasi-eikonal approximation used in the literature [803, 811. Also, the AGK technique allows one to calculate other quantities such as nuclear diffractive PDFs and fluctuations of multiplicity in non-diffractive DIS [803, 807, 812, both of which turn out to be sensitive to the pattern of the color fluctuations, see Section 5.4.

Our approach to nuclear shadowing assumes the applicability of the linear (in parton densities) leading-twist DGLAP approximation. Numerical studies indicate that the dominant contribution to nuclear shadowing in eq. (5.33) comes from the region of relatively large $\beta=Q^{2} /\left(M^{2}+Q^{2}\right)$ corresponding to the rapidity intervals $\leq 3$ for which the small$x$ approximation used in the BFKL-type approaches is not applicable. These approaches predict $\alpha_{\mathbb{P}}(0) \sim 1.25$, while the HERA experiments find $\alpha_{\mathbb{P}}(0) \sim 1.11 \approx \alpha_{\mathbb{P}}^{\text {soft }}(0)$ consistent with the expectations of the QCD aligned jet approximation 813 that we effectively implemented in the derivation of eq. (5.33).

## Non-perturbative approaches

## Hans J. Pirner

One of the challenges in QCD is the description and understanding of high-energy scattering on protons and nuclei. Even for high energies and large $Q^{2}$ in deep inelastic electron scattering a non-perturbative framework may be necessary. For the transverse structure function, the $q \bar{q}$ dipole in the photon can be large and the saturation scale $Q_{s}$ is small for the energies we discuss. In the following I will present the main features of such an
approach, which of course will also include the perturbative aspects.
The most important phenomenon observed in high-energy scattering is the rise of the total cross sections with increasing c.m. energy. While the rise is slow in hadronic reactions of large particles such as protons, pions, kaons, or real photons, it is steep if one small particle is involved such as an incoming virtual photon or an outgoing charmonium. This energy behavior is best seen in the proton structure function $F_{2}\left(x, Q^{2}\right)$. With increasing photon virtuality $Q^{2}$, the increase of $F_{2}\left(x, Q^{2}\right)$ towards small Bjorken $x$ becomes significantly stronger. It is tempting to test the growth of the structure function with nuclei. In the following I will summarize my work with Shoshi, Steffen and Dosch which is published in two main papers [814, 815]. For references to other work please see these two papers.

In the two-pomeron model of Donnachie and Landshoff, the energy dependence of the cross sections at high energies results from the exchange of a soft and a hard pomeron. The first dominates in hadron-hadron and $\gamma^{*} p$ reactions at low $Q^{2}$ and the second in $\gamma^{*} p$ reactions at high $Q^{2}$. The two pomerons may be related to a glueball trajectory, which is inherently non-perturbative, and a gluon ladder à la BFKL, which includes the perturbative aspects. The two-pomeron model, however, does not contain parton saturation nor unitarity effects. A model motivated by the concept of parton saturation is the one of Golec-Biernat and Wüsthoff which allows very successful fits to $\gamma^{*} p$ data, but cannot be applied to hadronhadron reactions. A successful description of dipole nucleon scattering which can be used for hadron-nucleon scattering and DIS with moderate $Q^{2}$ has been found 795 .

We have combined perturbative and non-perturbative QCD to compute high-energy reactions of hadrons and photons with special emphasis on saturation effects that manifest $S$-matrix unitarity 814. We follow the functional integral approach to high-energy scattering of Nachtmann, in which the $S$-matrix element factorizes into the universal correlation of two light-like Wegner-Wilson loops $S_{D D}$. The light-like Wegner-Wilson loops describe color dipoles given by the quark and antiquark in the meson or photon projectile and the quark and di-quark in the baryon target. This approach treats projectile and target symmetrically. $S$-matrix unitarity is respected as a consequence of a matrix cumulant expansion and the Gaussian approximation of the functional integrals. The resulting dipole cross sections do not show Glauber-like behavior with the dipole size as in the Golec-Biernat model. The loop-loop correlation function $S_{D D}$ is expressed in terms of the gauge invariant bi-local gluon field strength correlator integrated over two connected minimal surfaces. Due to the symmetric treatment of the two dipoles this formalism can explicitly investigate the dependence on the impact parameter of the two scattering partners.

The gluon field strength correlator has a non-perturbative and a perturbative component. The stochastic vacuum model of Dosch and Simonov is used for the non-perturbative low frequency background field and perturbative BFKL gluon exchange for the high frequency contributions. This combination allows us to describe long and short distance correlations in agreement with Euclidean lattice calculations of the static quark-antiquark potential with color-Coulomb behavior at short distances and confining linear rise at long distances. We have tried to model both components in AdS/QCD, but the long range looploop correlation cannot be established on a classical level, since the connecting surface in 5 dimensions breaks off at large distances 816.

Energy dependence in the loop-loop correlation function, $S_{D D}$, is introduced by hand in order to describe simultaneously the energy behavior in hadron-hadron, photon-hadron, and photon-photon reactions involving real and virtual photons as well. Motivated by the twoPomeron picture of Donnachie and Landshoff, we ascribe to the soft and hard component a weak and strong energy dependence, respectively. The parameter describing the energy
dependence of the perturbative correlation function is very large because we include multiple gluonic interactions. In ref. [814] we have considered not only the dependence of the dipole cross section on dipole size with increasing energy and the resulting $k_{t}$-saturation, but also the scattering amplitudes in impact parameter space, where the $S$-matrix unitarity imposes rigid limits on the impact parameter profiles such as the black disc limit. We present profile functions for longitudinal photon-proton scattering that provide an intuitive geometrical picture for the energy dependence of the cross sections. The profile function first becomes greyer, turns black and then increases in transverse size. Using a leading-twist NLO DGLAP relation, we estimated the impact parameter dependent gluon distribution of the proton $x G\left(x, Q^{2},\left|\vec{b}_{\perp}\right|\right)$ from the profile function for longitudinal photon-proton scattering. We have not found saturation of the profile function at HERA energies, but at higher energies, $x G\left(x, Q^{2},\left|\vec{b}_{\perp}\right|\right)$ does saturate as a manifestation of the $S$-matrix unitarity.

In the same framework, we have studied the unintegrated gluon distribution $x G\left(x, k_{t}\right)$ as a function of transverse momentum $k_{t}$ for increasing energies 815. To obtain the unintegrated gluon distribution, one uses the possibility to rewrite the non-perturbative scattering of an artificial external dipole as a superposition of perturbative contributions. In other words the string of the projectile dipole can be decomposed mathematically in a superposition of dipoles of smaller sizes, from which $x G\left(x, k_{t}\right)$ can be extracted.

The long range confining character of the non-perturbative field strength correlators determines the low $k_{t}$ behavior of the gluon structure function of the hadron as $x G\left(x, k_{t}\right) \propto$ $1 / k_{t}$. In the low momentum limit, $x G\left(x, k_{t}\right) \cdot k_{t}$ converges towards a constant independent of $x$, related to the size of the hadron. The cross-over from the non-perturbative region to the perturbative region occurs at around $k_{t}=1 \mathrm{GeV}$ at $x$-values $10^{-4}<x<10^{-2}$.

On a more fundamental level, we have analysed correlations of Wilson lines in vacuum as one approaches the light cone from space-like distances [817]. The dominant terms of the near light cone Hamiltonian for the Wilson lines define a field theory in $2+1$ dimensions. In the limit of small x , the $\mathrm{SU}(3) \mathrm{QCD}$ for Wilson lines reduces to a critical $\mathrm{Z}(3)$ theory with a diverging correlation length $\xi(x) \propto x^{-1 /\left(2 \lambda_{2}\right)}$ where the exponent $\lambda_{2}=2.52$ is obtained from the center group $\mathrm{Z}(3)$ of $\mathrm{SU}(3)$. We conjecture that the dipole wave function of the virtual photon behaves as the correlation function of Wilson lines in the vacuum. For transverse sizes smaller than the correlation size it scales like $\Psi \propto 1 /\left(x_{t}\right)^{1+n}$ with $n=0.04$ and for distances larger than the correlation length it decays exponentially which makes this region negligible. For $F_{2}$ we integrate the square of the photon wave function weighted with a dipole proton cross section of fixed size $R_{0}$ independent of x. All the energy dependence is absorbed into the photon. Because of the approximate conformality of the dipole wave function ( $n \approx 0$ ), the result depends only on $R_{0}^{2} / \xi(x)^{2} \propto R_{0}^{2} x^{1 / \lambda_{2}}$, i.e. the saturation scale varies as as $Q_{s}^{2}=Q\left(x_{o}\right)^{2}(x 0 / x)^{1 / \lambda_{2}}$. The critical index in this theory is a characteristic feature of $Z(3)$ theory i.e. the center group of $\mathrm{SU}(3)$ in an external field given by the light quarks. This is very different from the perturbative color glass condensate where $Q_{s}$ depends on the running coupling similarly to the power behaviour of BFKL.

### 5.3 Inclusive DIS ( $\mathrm{F}_{2}, \mathrm{~F}_{L}, \mathrm{~F}_{2}^{c}$ )

## Estimates of higher twist in deep inelastic nucleon and nucleus scattering

Joachim Bartels, Krzysztof Golec-Biernat and Leszek Motyka

A deeper understanding of the transition region at low $Q^{2}$ and small $x$ in deep inelastic electron proton scattering has been one of the central tasks of HERA physics. It will be one of the key questions to be addressed by a future Electron Ion Collider. Approaching this transition region from the perturbative side, one expects to see the onset of corrections to the successful DGLAP description, based upon leading twist operators in QCD. The twist expansion defines a systematic approach to the short distance limit probed in deep inelastic scattering. The study of higher-twist corrections therefore provides an attractive route for investigating the region of validity of the leading twist DGLAP evolution equations.

The validity of the leading-twist QCD evolution equations is based upon the fact that, for sufficiently large $Q^{2}$ and not too small $x$, the gluons inside the proton are dilute. The DGLAP evolution equations, however, predict that, at small $x$ and low $Q^{2}$, the gluon density grows. As a result, the gluons start to interact and the gluon density eventually saturates. The onset of saturation is encoded in the saturation scale, $Q_{\text {sat }}^{2}(x)$.

The investigation of saturation is of highest importance for our understanding of QCD. Saturation can be viewed as a first step of entering the strong interaction region. While the QCD coupling constant is still small, saturation phenomena probe nonlinear dynamics of the gluon sector which plays a crucial role in many areas of strong interactions. It is expected that saturation effects in deep inelastic scattering on a nucleus are enhanced in comparison with deep inelastic scattering on a proton. In the former case, the incoming photon 'sees' the gluons of many nucleons, whereas in the case of a single nucleon, one has to go to smaller $x$ values (higher energies) in order to reach the same gluon density.

A brief discussion of the connection between saturation and the twist expansion has been given in 818]. Whereas in the GBW model [83, 819 ] there is a rather direct classification of eikonal-type exchanges of gluon ladders in terms of twist quantum numbers, in saturation models based upon the nonlinear BK-equation [85, 820] a twist decomposition is much less obvious. In the following we present some numerical estimates of higher-twist contributions, using the improved version of the GBW model 821 .

The method: The theory of higher-twist operators and their evolution equations has been outlined in 822]: in leading order, the higher-twist evolution equations are described by the nonforward DGLAP splitting functions, and there is a particular pattern of mixing between different operators of the same twist. In the same way as for leading twist, a numerical analysis of higher twists requires initial conditions for the set of evolution equations, which have to be adjusted to data. In 818 the magnitude of higher-twist corrections was evaluated in a slightly different way. Starting from the observation that within the GBW saturation model the multiple exchanges of leading-twist gluon ladders can be put into a one-toone correspondence with contributions of definite twist quantum numbers, it is possible to arrive at quantitative estimates of the leading-twist contributions and corrections due to twist $\tau=4,6, \ldots$. Details have been described in [818] and will not be repeated here.

While the analysis in [818] was performed for the case of $e+p$ scattering, it is straightforward to extend it to electron-nucleus scattering. Assuming a cylindrical nucleus with a characteristic size $R_{A} \approx A^{1 / 3} R_{p}$ (with $R_{p}$ being the proton radius), we simply replace the


Figure 5.20. Higher-twist contribution estimate for $F_{2}$ (left) and $F_{L}$ (right) of the proton.
dipole-proton cross section (eq.(42) in [818])

$$
\begin{equation*}
\sigma_{\text {dipole-proton }}=\sigma_{0}\left(1-\exp \left(-\Omega\left(x, r^{2}\right)\right)\right) \tag{5.34}
\end{equation*}
$$

by the dipole-nucleus cross section

$$
\begin{equation*}
\sigma_{\text {dipole-nucleus }}=A^{2 / 3} \sigma_{0}\left(1-\exp \left(-A^{1 / 3} \Omega\left(x, r^{2}\right)\right)\right) \tag{5.35}
\end{equation*}
$$

where $\Omega\left(x, r^{2}\right)$ is the eikonal function given in [818]. With the parameters from [818] we simply repeat the electron proton calculations for electron gold scattering, using the modified dipole cross section formula in (2).


Figure 5.21. Higher-twist contribution estimate for $F_{2}$ (left) and $F_{L}$ (right) of the gold nucleus.
Numerical results: The numerical results for $F_{2}$ and $F_{L}$ are shown in Fig. 5.20 for the proton, and Fig. 5.21 for the gold nucleus. In each figure we show, on the l.h.s in a 3dimensional view, the ratio of the higher-twist corrections and the full structure function as a fucntion of $x$ and $Q^{2}$,

$$
\begin{equation*}
\text { ratio }=\frac{F_{2, L}^{(\text {total })}-F_{2, L}^{(\tau=2)}}{F_{2, L}^{\text {(total })}} . \tag{5.36}
\end{equation*}
$$

The r.h.s. shows the projection onto the $\left(\log x, \log Q^{2}\right)$ plane: the lines belong to fixed values of the ratio (5.36). One recognizes the general trend: the corrections are getting larger when $x$ and $Q^{2}$ decrease (moving towards the lower left corner). For given $x$ and $Q^{2}$, the corrections for the longitudinal structure functions are larger than for $F_{2}$. This is a consequence of the sign structure of the corrections in $F_{L}$ and $F_{T}$ : twist four corrections to $F_{L}$ and $F_{T}$ have opposite signs, and in the analysis [818] of $F_{2}=F_{T}+F_{L}$ a strong cancellation has been found. This explains the small higher twist contribution for $F_{2}$.

One also recognizes the general trend that for gold, all corrections are larger than for the proton. Finally, the corrections to $F_{L}$ are negative and those to $F_{2}$ are mostly positive. In the case of the proton $F_{2}$ there is a change in sign in the region of very small values of $Q^{2}$ : this again is a consequence of the sign structure of the twist corrections to $F_{T}$ and $F_{L}$.

Conclusions: Our numerical analysis confirms that, in general, the structure functions $F_{L}$ are more sensitive to higher-twist corrections than $F_{2}$ which, because of the sign structure in the twist 4 corrections, seems to much better "protected" against higher twist. Also, nuclear targets are more sensitive to higher twist corrections relative to the proton. In view of these results, it seems clear that in a future electron-ion collider, the measurement of $F_{L}$ is of vital importance in the search for saturation.

## Strength of nonlinear effects in nucleons and nuclei

## Tuomas Lappi

The effects of nonlinearity and unitarity in small $x$ DIS are most clearly visible in the dipole framework. We denote $\mathcal{N}\left(x, \mathbf{b}_{T}, \mathbf{r}_{T}\right)$ the imaginary part of the scattering amplitude for a dipole of size $\mathbf{r}_{T}$ and rapidity $y=\ln (1 / x)$ to scatter off the target at impact parameter $\mathbf{b}_{T}$. The total dipole cross section is given by twice the integral of $\mathcal{N}\left(x, \mathbf{b}_{T}, \mathbf{r}_{T}\right)$ over the impact parameter. While the formal unitarity limit would be for $\mathcal{N}$ to lie between 0 and 2 , in practice the reasonable physical area is between 0 (no scattering) and 1 (complete absorption or the black disk limit). The typical value of the dipole scattering amplitude therefore serves as a good measure of the degree of nonlinearity of the scattering process.


Figure 5.22. The saturation scale in a proton and Ca and Au nuclei as a function of $b / b_{\text {med }}$, where $b_{\text {med }}$ is the median impact parameter probed in inclusive DIS at $x=0.001$ and $Q^{2}=1 \mathrm{GeV}^{2}$.

As the total cross section depends on the integral of the scattering amplitude over the impact parameter, statements about the magnitude of the scattering amplitude depend on the profile of the target in $\mathbf{b}_{T}$. The $\mathbf{b}_{T^{-}}$ depdendence for the scattering amplitude on a nucleon is, however, very much constrained by the $t$-dependence of exclusive vector meson production. Using this information, in addition to the total cross section, results in the two commonly used $\mathbf{b}_{T}$-dependent dipole amplitude parametrizations that we will use here, the IPsat and bCGC models 600, 823, 824]. They have successfully been used to describe HERA data on the inclusive cross section, exclusive vector meson production and diffractive structure functions 825 .

The saturation scale: To a first approximation the impact parameter dependence of the nuclear scattering amplitude can then be obtained by combining the nucleon one with basic knowledge of nuclear geometry in a Glauber-like treatment (see e.g. Refs. [826, 827] for details). This yields a characteristic pattern of nuclear suppression (shadowing) of the inclusive cross section, a nuclear enhancement of diffraction to small mass states and a
suppression in diffraction to large masses (small $\beta$ ) 825].
One way of quantifying the importance of nonlinear effects is to compare the value of the ( $\mathbf{b}_{T}$ and $x$-dependent) saturation scale $Q_{\mathrm{s}}^{2}$ to the virtuality $Q^{2}$ of the process. The saturation scale is defined as the inverse of the dipole size at which the scattering amplitude $\mathcal{N}$ reaches some specific value defined by convention. For $Q^{2} \gg Q_{\mathrm{s}}^{2}$ one is in the dilute limit and for $Q^{2} \sim Q_{\mathrm{s}}^{2}$ nonlinear effects become important. A naive argument of the $A$ dependence of the saturation scale for nuclei would give $Q_{\mathrm{s} A}^{2} \sim A^{1 / 3}$. The importance of a realistic impact parameter dependence for nuclei was discussed in more detail in Ref. 826], where it was found that this dependence is indeed true to a very good approximation, but the picture is more intricate than that. For the center of a nucleus vs. the center of a proton the saturation scale is suppressed by a geometrical factor $\sim 0.3 \approx R_{p}^{2} A^{2 / 3} / R_{A}^{2}$. Both a nucleon and a nucleus have a dilute edge at large impact parameters. The thickness of this edge is determined by confinement scale physics and is thus of the same order for both. The proton is, however, a much smaller object and therefore the dilute edge region is responsible for a much larger fraction of the total cross section than in a nucleus. One way to see this is to look at the saturation scale at the median impact parameter contributing to the inclusive cross DIS cross section. The value of $Q_{\mathrm{s}}^{2}\left(b_{\text {med }}\right)$ is $\sim 35 \%$ of the value at $b=0$ for a proton, but $\sim 70 \%$ for a gold nucleus (see Fig. [5.22, [826]).


Figure 5.23. Longitudinal mean scattering amplitude $\langle\mathcal{N}\rangle_{L}$ for a proton (left) and a a gold nucleus (right) with the IPsat parametrization (first row) and bCGC parametrization (second row).

The mean scattering amplitude: An alternative way of assessing the typical values of the scattering amplitude is to calculate its expectation value weighted by the cross section
of a particular process. We thus define the mean scattering amplitude as

$$
\begin{equation*}
\langle\mathcal{N}\rangle_{T, L}=\frac{\int \mathrm{d}^{2} \mathbf{r}_{T} \int_{0}^{1} \mathrm{~d} z\left|\Psi_{L, T}^{\gamma^{*}}\right|^{2} \int \mathrm{~d}^{2} \mathbf{b}_{T} \mathcal{N}^{2}\left(x, \mathbf{b}_{T}, \mathbf{r}_{T}\right)}{\int \mathrm{d}^{2} \mathbf{r}_{T} \int_{0}^{1} \mathrm{~d} z\left|\Psi_{L, T}^{\gamma^{*}}\right|^{2} \int \mathrm{~d}^{2} \mathbf{b}_{T} \mathcal{N}\left(x, \mathbf{b}_{T}, \mathbf{r}_{T}\right)} . \tag{5.37}
\end{equation*}
$$

This will yield a value between 0 and 1 for all points in the $Q^{2}, x$-plane. Note that although in principle $\langle\mathcal{N}\rangle$ varies between 0 and 1 , the maximal value for a Gaussian $\mathbf{b}_{T}$-distribution, which describes the proton very well, is only $1 / 2$. The longitudinal and transverse structure functions probe a slightly different distribution of dipole sizes $r$, with the longitudinal structure function showing a stronger $Q^{2}$-dependence. The same quantities can easily be computed also for charm quarks only.


Figure 5.24. The mean scattering amplitude $\langle\mathcal{N}\rangle_{\text {tot }}$ for the total cross section for a proton (left) and a a gold nucleus (right) with the bCGC parametrization.

Figure 5.23 shows the mean scattering amplitude probed in the longitudinal total cross section in a proton and a gold nucleus in the IPsat model. The characteristic feature of the eikonalized DGLAP-evolved gluon distribution in this parametrization is the fact that the $x$-dependence becomes faster at higher energies. The same quantity for the bCGC cross section is plotted in fig. 5.23, Here one sees the characteristic constant energy dependence $Q_{\mathrm{s}}^{2} \sim x^{-\lambda}$ in the bCGC parametrization leading to straight lines of constant $\mathcal{N}$ in a $\log -\log$ plot. The amplitude weighted by the total cross section is shown in Fig. 5.24 for the IPsat parametrization. It shows a slower $Q^{2}$-dependence than the longitudinal one, connected with the well-known fact that the longitudinal structure function is more sensitive to higher-twist effects than the total one.

In all plots for protons we have shown the kinematical limits for HERA and the EIC ( 325 GeV proton on 30 GeV electron with $y<0.9$ ) and in the nucleus plots for the EIC ( 130 A GeV nucleus on 30 GeV electron with $y<0.9$ ) and lower energy mEIC option ( $130 A \mathrm{GeV}$ nucleus on 5 GeV electron with $y<0.9$ ). The comparison between nuclei and protons is striking. In the IPsat parametrization, as is typical of DGLAP evolution, the energy dependence at the initial small $Q^{2}$-scale is very slow. Thus the lower energy of the EIC compared to HERA would be insignificant in face of the effect of using nuclei. A value of $\langle\mathcal{N}\rangle_{\text {tot }}$ of 0.3 could, for example, be reached at $Q^{2}=4 \mathrm{GeV}^{2}$ at the EIC vs. $Q^{2}=1 \mathrm{GeV}^{2}$ at HERA; much more safely in the weak coupling regime. With nuclei the EIC could, at $Q^{2}=1 \mathrm{GeV}$, reach values of $\langle\mathcal{N}\rangle_{L} \approx 0.5$ that are simply inaccessible in an ep collider at practically any energy for an approximately Gaussian proton profile.

Acknowledgments: M. Diehl came up with the idea of visualizing the strength of the nonlinear effects in the way presented here.

## Nuclear PDFs and deviations from DGLAP evolution

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In this contribution we present a preliminary analysis which aims at determining the potential of the EIC to measure gluon shadowing and anti-shadowing and its sensitivity to saturation dynamics.

The input for this analysis is the EIC pseudo data for the inclusive DIS cross section in two scenarios, a medium energy EIC $(\sqrt{s}=$ $12,17,24,32,44 \mathrm{GeV}$, denoted by stage I) and a full energy $\operatorname{EIC}(\sqrt{s}=63,88,124 \mathrm{GeV}$, stage II), with $0.004<y<0.8$ in either case. The kinematic coverage is summarized in Fig. 5.25. The pseudo-data was generated starting from $e+p$ and $e+n$ cross sections computed using the central values of the NNPDF2.0 parton distributions [47. An integrated luminosity of $4 \mathrm{fb}^{-1}$ was assumed for all energies, and the pseudodata has been corrected for the expected statistical fluctuations. For most of the $x$ range the resulting statistical errors are negligible compared to the assumed $2 \%$ systematic error. Nuclear effects have been included in a $K$-factor approx-


Figure 5.25. Kinematical coverage of the pseudo-data included in the NNPDF analysis of the EIC e +Pb cross-sections, both for stage I and for stage II. Possible kinematical cuts relevant to the study of the onset of non-linear phenomena are also shown. imation, so that the longitudinal and transverse cross sections in ${ }^{208} \mathrm{~Pb}$ can be expressed in terms of the proton cross sections as

$$
\begin{equation*}
\sigma_{T, L}^{\mathrm{Pb}}\left(x, Q^{2}, y\right)=K_{T, L}^{\lambda}\left(x, Q^{2}, y\right) \sigma_{T, L}^{\mathrm{p}}\left(x, Q^{2}, y\right) \tag{5.38}
\end{equation*}
$$

where the label $\lambda$ sets the intensity of the assumed saturation effects, and $\lambda=1$ corresponds to the nominal saturation in the IP Non-sat model [600]. In particular, the $K$-factor in Eq. (5.38) is given by the following piece-wise expression. For small $x, x \leq 0.01$,

$$
\begin{equation*}
K_{T, L}^{\lambda}=\frac{2}{\left\langle\sigma_{q \bar{q}}\right\rangle_{T, L}} \int d^{2} b\left\langle\left(1-e^{-\lambda \frac{1}{2} A \sigma_{q \bar{q}} T_{A}(b)}\right)\right\rangle_{T, L}, \tag{5.39}
\end{equation*}
$$

where $\sigma_{q \bar{q}}$ is the dipole cross section in the IP Non-sat model (we assume for simplicity that in the EIC kinematic range there is no saturation at the proton level, and search for the nuclear medium-induced saturation); $T_{A}(b)=\int d z \rho_{A}(b, z)$, where $\rho_{A}(b, z)$ is the nuclear density normalized to unity; the brackets $\langle\ldots\rangle_{T, L}$ stand for the integration with the wave function squared of a virtual photon with transverse or longitudinal polarization, respectively. In the $0.01 \leq x \leq 0.1$ interval, we assume that $K_{T, L}^{\lambda}$ increases linearly from the value given by Eq. (5.39) at $x=0.01$ up to $K_{T, L}^{\lambda}=1$ at $x=0.1$. For $x>0.1$, we assumed that $K_{T, L}^{\lambda}$ is equal to the ratio of the nuclear to free nucleon structure functions, $F_{2 A}\left(x, Q^{2}\right) /\left[A F_{2 N}\left(x, Q^{2}\right)\right]$, which is given by the leading-order parameterization of Ref. [828]

Nuclear parton distributions are then determined by a Next-to-Leading Order QCD fit of the pseudo-data within the NNPDF framework [681, 47]. The kinematic cuts used to ensure the validity of DGLAP evolution are $Q^{2} \geq 2 \mathrm{GeV}^{2}$ and $W^{2} \geq 12.5 \mathrm{GeV}^{2}$. In this preliminary study, we consider pseudo-data for Pb targets only, and postpone discussion of the dependence of the nuclear PDFs on $A$ to a future investigation. In the collinear factorization approximation, Pb structure functions are related to Pb parton distributions in the same way as in the proton case (see Section 5.7 and Ref. [829). We also assumed for simplicity the Pb nucleus to be isoscalar, so that the structure functions depend only on three independent nuclear PDFs: the singlet quark PDF, $\Sigma^{\mathrm{Pb}}\left(x, Q^{2}\right)$, the gluon PDF $g^{\mathrm{Pb}}\left(x, Q^{2}\right)$, and the strange PDF; the latter was furthermore set to be a fixed fraction of the singlet PDF.

Now we discuss some preliminary results of the nuclear PDF fits. We show in Fig. 5.26 the singlet and the gluon PDFs at the initial scale $Q^{2}=2 \mathrm{GeV}^{2}$ obtained using only stage I data for $\mathrm{e}+\mathrm{Pb}$ collisions, and then adding the stage II data. To illustrate the accuracy that the EIC can reach in the determination of nuclear PDFs we show in Fig. 5.27 their relative uncertainties alongside those of the proton's NNPDF2.0 47] combined with those of the EPS09 nuclear modifications [40] for ${ }^{208} \mathrm{~Pb}$, which allows a comparison of the relative error bands. Since the restrictive EPS09 parametrization may underestimate the nuclear uncertainties outside the region where data is presently available, notably at $x \lesssim 0.01$, we added the relative NNPDF2.0 and EPS09 relative uncertainties linearly for a conservative estimate of the total uncertainty.


Figure 5.26. The quark singlet (left plot) and the gluon PDFs (right plot) in Pb at the initial evolution scale $Q_{0}^{2}=2 \mathrm{GeV}^{2}$, for stage I and stage I+II.

The measurement of the nuclear modifications of the gluon are one of the most important measurements at the EIC, as this quantity is essentially unknown from present data. Inclusive cross sections are sensitive to the gluon distribution both via scaling violations and, to a lesser extent, through the longitudinal structure function accessed through the proposed $\sqrt{s}=12-124 \mathrm{GeV}$ energy scan. From Fig. 5.26 we see that one can determine, with reasonable accuracy, the gluon shadowing down to $x \sim 10^{-3}$ in stage II and down to $x \sim 10^{-2}$ in stage I. The better capabilities of stage II stem both from its greater lever arm in $Q^{2}$ and its coverage of smaller values of $x$, see Fig. 5.25. In particular, the precision of the Pb gluon in Stage II at small $x$ is comparable to estimates from global proton fits. On top of this, at the EIC it will be possible to study gluon anti-shadowing, EMC and Fermi motion effects with much better accuracy than afforded by current global nuclear fits (see Sections 5.7 and 5.7 We can also see that EIC will measure accurately the sea quark shadowing, and that nuclear modifications of light quarks at large $x$ could be measured a precision similar or even better than for the proton case.


Figure 5.27. The relative uncertainty in the quark singlet (two upper panels) and the gluon PDFs in Pb (two lower panels) at the initial evolution scale $Q_{0}^{2}=2 \mathrm{GeV}^{2}$, with stage I and stage $\mathrm{I}+\mathrm{II}$ data. Results are shown on linear (left plot) and logarithmic (right plot) scales. For reference, the analogous results for the Pb PDFs using NNPDF2.0+EPS09 parametrizations are also shown.

This analysis was based on the validity of collinear factorization for nuclei, and the validity of linear DGLAP evolution in $Q^{2}$. However, at small enough $x$ and $Q^{2}$, deviations from linear fixed order DGLAP evolution are expected to appear, e.g., due to small- $x$ resummation effects 830] or gluon saturation, see Section 5.2. In heavy nuclei, the effects due to gluon saturation are boosted to higher $Q^{2}$ and $x$ by the atomic number; one then has the possibility of experimentally separating small- $x$ and saturation effects, which is not be possible with HERA $e+p$ data.

In Refs. [720, 831] a general strategy was presented to quantify potential deviations from NLO DGLAP evolution, which was then applied to proton HERA data. In a global PDF fit, deviations from DGLAP in the data can be hidden in a distortion of parton distributions; however, these can be singled out by determining undistorted PDFs from data in regions where such effects are expected to be small. In more detail, one can fit PDFs using data at large $x$ and $Q^{2}$, where DGLAP is likely to hold with high accuracy, and then evolving them down in the $Q^{2}$ region where deviations are expected to arise. DGLAP deviations can then be quantitatively determined by comparing calculations to data in this region, which were not used in the PDF determination.

This approach can be applied as well to the nuclear case. From simple theoretical arguments about the energy and $A$ dependence of the saturation scale (see Section [5.2), we expect deviations from linear evolution to appear when $Q^{2} \lesssim \bar{Q}^{2}(A \bar{x} / x)^{\frac{1}{3}}$, where $\bar{x}$ is a reference value, say $\bar{x}=10^{-3}$, and $\bar{Q}^{2}$ is the scale where DGLAP evolution at $\bar{x}$ would be broken in the proton. Note however that the $A$-dependence of the saturation scale may in fact be tamed by the leading twist nuclear shadowing, see Section 5.2. While saturation models may give an indication of the value of $\bar{Q}^{2}$, we wish to determine this scale in a model independent way as the scale at which deviations from DGLAP evolution can be detected from EIC nuclear target (pseudo-)data. The unsafe region for DGLAP evolution can also be
written as $Q^{2} \lesssim Q_{c}^{2} x^{-\frac{1}{3}}$ with $Q_{c}^{2}$ some constant setting the strength of the deviations from DGLAP. In Refs. 720,831 the range $Q_{c}^{2} \in[0.5,1.5] \mathrm{GeV}^{2}$ was considered for the proton case; in the nuclear case this range should be rescaled by a factor $A_{\mathrm{Pb}}^{1 / 3} \approx 6$. Typical values of these kinematical cuts for the Pb nucleus are shown in Fig. 5.25.



Figure 5.28. The Pb structure function $F_{2}^{\mathrm{Pb}}\left(x, Q^{2}\right)$ at $Q^{2}=3 \mathrm{GeV}^{2}$ from the analysis of the EIC stage I (left plot) and stage I+II (right plot) simulated data with $\lambda=1$, without kinematical cuts and with cuts using $Q_{c}^{2}=1.5 A_{\mathrm{Pb}}^{1 / 3} \sim 9$.

We show in Fig. 5.28 a representative result of the fits to the EIC pseudo-data after applying the cut with $\bar{Q}^{2}=1.5 A_{\mathrm{Pb}}^{1 / 3} \sim 9$, compared to the reference uncut fits to stages I and $\mathrm{I}+\mathrm{II}$ pseudo-data with $\lambda=1$. As expected when data is removed the uncertainties in the physical observables become much larger, but one can still see a systematic downwards shift in the central value, which is the signature of the departure from linear evolution [720, 831]. Note that this signal is already apparent with stage I data only, although its statistical significance might be marginal.

We plan to systematically explore the sensitivity of the EIC to non-linear dynamics using this technique, by optimizing the kinematical cuts for different values of the saturation scale used to generate the pseudo-data, exploit the interplay between the $F_{2}^{\mathrm{Pb}}$ and $F_{L}^{\mathrm{Pb}}$ structure functions, and quantitatively measuring the statistical significance of the signal. This will determine in a fairly model-independent way the smallest saturation scale that can be detected at the EIC in either stage I or stage II.

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## Constraining the nuclear gluon distribution using inclusive observables

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Data from HERA allow for a good determination of the gluon density of the proton. A much harder task has been to determine the gluon distribution of nucleons bound in a nucleus, the nuclear gluon distribution $\left(x g^{A}\left(x, Q^{2}\right)\right)$. Existing data, taken over a wide kinematic range $10^{-5} \leq x \leq 0.1$ and $0.05 \mathrm{GeV}^{2} \leq Q^{2} \leq 100 \mathrm{GeV}^{2}$, show a systematic reduction of the nuclear structure function $F_{2}^{A}\left(x, Q^{2}\right) / A$ with respect to the free nucleon structure function $F_{2}^{N}\left(x, Q^{2}\right)$. This phenomenon is known as the nuclear shadowing effect and is associated to the modification of the target parton distributions so that $x q^{A}\left(x, Q^{2}\right)<$ $A x q^{N}\left(x, Q^{2}\right)$, as expected from a superposition of $e p$ interactions. The modifications depend on the parton momentum fraction: for momentum fractions $x<0.1$ (shadowing region)
and $0.3<x<0.7$ (EMC region), a depletion is observed in the nuclear structure functions. These two regions are bridged by an enhancement known as antishadowing for $0.1<x<$ 0.3 . The experimental data for the nuclear structure function determine the behaviour of the nuclear quark distributions, while the behaviour of the nuclear gluon distribution is indirectly determined using the momentum sum rule as a constraint and/or studying the $\log Q^{2}$ slope of the ratio $F_{2}^{S n} / F_{2}^{C}$. Currently, the behaviour of $x g^{A}\left(x, Q^{2}\right)$ at small $x$ (high energy) is completely uncertain as shown in Fig. 5.29, where we present the ratio $R_{g}=x g^{A} /\left(A . x g^{N}\right)$, for $A=208$, predicted by four different groups which realize a global analysis of the nuclear experimental data using the DGLAP evolution equations in order to determine the parton densities in nuclei. In particular, the magnitude of shadowing and the presence or not of the antishadowing effe

In this contribution we study the behaviour of the nuclear longitudinal structure function $F_{L}^{A}$ and the charm structure function $F_{2}^{c, A}$ and analyse the possibility to constrain the nuclear effects present in $x g^{A}$ using these inclusive observables (For more details and references see Ref. [832]).

## $F_{L}^{A}$ and $F_{2}^{c, A}$ in the collinear formal-

 ism: The longitudinal structure function in deep inelastic scattering is one of the observables from which the gluon distribution can be unfolded. In the collinear formalism, $F_{L}$ is described in terms of the AltarelliMartinelli equation

Figure 5.29. The ratio $R_{g}=x g^{A} / A \cdot x g^{N}$ predicted by the EKS, DS, HKN and EPS parametrizations for $A=208$ and $Q^{2}=2.5 \mathrm{GeV}^{2}$.

$$
\begin{equation*}
F_{L}\left(x, Q^{2}\right)=\frac{\alpha_{s}\left(Q^{2}\right)}{2 \pi} x^{2} \int_{x}^{1} \frac{d y}{y^{3}}\left[\frac{8}{3} F_{2}\left(y, Q^{2}\right)+4 \sum_{q} e_{q}^{2}\left(1-\frac{x}{y}\right) y g\left(y, Q^{2}\right)\right] \tag{5.40}
\end{equation*}
$$

At small $x$, the second term with the gluon distribution is the dominant one. This expression can be reasonably approximated by $F_{L}\left(x, Q^{2}\right) \approx 0.3 \frac{4 \alpha_{s}}{3 \pi} x g\left(2.5 x, Q^{2}\right)$, which demonstrates the close relation between the longitudinal structure function and the gluon distribution. Therefore, we expect the longitudinal structure function to be sensitive to nuclear effects.

In order to estimate the charm contribution to the structure function we treat the charm quark as a heavy quark and estimate its contribution by fixed-order perturbation theory. This involves the computation of the boson-gluon fusion process. A $\bar{c} \bar{c}$ pair can be created by boson-gluon fusion when the squared invariant mass of the hadronic final state is $W^{2} \geq 4 m_{c}^{2}$. Since $W^{2}=\frac{Q^{2}(1-x)}{x}+M_{N}^{2}$, where $M_{N}$ is the nucleon mass, the charm production can occur well below the $Q^{2}$ threshold, $Q^{2} \approx 4 m_{c}^{2}$, at small $x$. The charm contribution to the proton/nucleus structure function, in leading order (LO), is given by

$$
\begin{equation*}
\frac{1}{x} F_{2}^{c}\left(x, Q^{2}, m_{c}^{2}\right)=2 e_{c}^{2} \frac{\alpha_{s}\left(\mu^{\prime 2}\right)}{2 \pi} \int_{a x}^{1} \frac{d y}{y} C_{g, 2}^{c}\left(\frac{x}{y}, \frac{m_{c}^{2}}{Q^{2}}\right) g\left(y, \mu^{\prime 2}\right), \tag{5.41}
\end{equation*}
$$

where $a=1+\frac{4 m_{c}^{2}}{Q^{2}}$ and the factorization scale $\mu^{\prime}$ is assumed $\mu^{\prime 2}=4 m_{c}^{2} . C_{g, 2}^{c}$ is the coefficient


Figure 5.30. Ratios $R_{g}, R_{C}$ and $R_{L}$ for the four considered nuclear parametrizations, $Q^{2}=2.5$ $\mathrm{GeV}^{2}$ and $A=208$.
function given by

$$
\begin{align*}
C_{g, 2}^{c}\left(z, \frac{m_{c}^{2}}{Q^{2}}\right) & =\frac{1}{2}\left\{\left[z^{2}+(1-z)^{2}+z(1-3 z) \frac{4 m_{c}^{2}}{Q^{2}}-z^{2} \frac{8 m_{c}^{4}}{Q^{4}}\right] \ln \frac{1+\beta}{1-\beta}\right. \\
& \left.+\beta\left[-1+8 z(1-z)-z(1-z) \frac{4 m_{c}^{2}}{Q^{2}}\right]\right\} \tag{5.42}
\end{align*}
$$

where $\beta=1-\frac{4 m_{c}^{2} z}{Q^{2}(1-z)}$ is the velocity of one of the charm quarks in the boson-gluon center-of-mass frame. Therefore, in leading order, $\mathcal{O}\left(\alpha_{s}\right), F_{2}^{c}$ is directly sensitive only to the gluon density via the well-known Bethe-Heitler process $\gamma^{*} g \rightarrow c \bar{c}$. The dominant uncertainty in the QCD calculations arises from the uncertainty in the charm quark mass. In this contribution we assume $m_{c}=1.5 \mathrm{GeV}$.

The nuclear ratios: Let us now study the behaviour of the nuclear longitudinal structure function $F_{L}^{A}$ and the charm structure function $F_{2}^{c, A}$ and analyze the possibility to constrain the nuclear effects present in $x g^{A}$ using these inclusive observables. We estimate the normalized ratios

$$
\begin{equation*}
R_{L}\left(x, Q^{2}\right)=\frac{F_{L}^{A}\left(x, Q^{2}\right)}{A F_{L}^{p}\left(x, Q^{2}\right)} \quad \text { and } \quad R_{C}\left(x, Q^{2}\right)=\frac{F_{2}^{c, A}\left(x, Q^{2}\right)}{A F_{2}^{c, p}\left(x, Q^{2}\right)} \tag{5.43}
\end{equation*}
$$

considering four distinct parametrizations for the nuclear gluon distributions and compare their behaviour with those predicted for the ratio $R_{g}=x g^{A} / A x g^{N}$.

In Fig. 5.30 we present our results. Firstly, let us discuss the small- $x$ region, $x \leq 10^{-3}$, determined by shadowing effects. We observe that $R_{L}$ practically coincides with $R_{g}$ for all parametrizations and for the two values of $Q^{2}$ considered. This suggests that shadowing effects can be easily constrained in an $e A$ collider by measuring $F_{L}$. This conclusion is, to a good extent, model independent. On the other hand, the ratio $R_{C}$ gives us an upper
bound for the magnitude of the shadowing effects. For example, if it is found that $R_{C}$ is equal to $\approx 0.6$ at $x=10^{-4}$ and $Q^{2}=2.5 \mathrm{GeV}^{2}$ the nuclear gluon distributions from DS and HKN parametrizations are very large and should be modified. Considering now the kinematical range of $x>10^{-3}$ we can analyse the correlation between the behaviour of $R_{L}$ and $R_{C}$ and the antishadowing present or not in the nuclear gluon distribution. Similarly to what is observed at small values of $x$, the behaviour of $R_{L}$ is very close to the $R_{g}$ one in the large- $x$ range. In particular, the presence of antishadowing in $x g^{A}$ directly implies an enhancement in $F_{L}^{A}$. It is almost $10 \%$ smaller in magnitude that the enhancement predicted for $x g^{A}$ by the EKS and EPS parametrizations. Inversely, if we assume the non-existence of the antishadowing in the nuclear gluon distribution at $x<10^{-1}$, as in the DS and HKN parametrizations, no enhancement will be present in $F_{L}^{A}$ in this kinematical region. Therefore, it suggests that also the antishadowing effects can be easily constrained in an $e A$ collider measuring $F_{L}$. On the other hand, in this kinematical range the behavior of $R_{C}$ is distinct of $R_{g}$ at a same $x$. However, we observe that the behavior of $R_{C}$ at $x=10^{-2}$ is directly associated to $R_{g}$ at $x=10^{-1}$. In other words, the antishadowing is shifted in $R_{C}$ by approximately one order of magnitude in $x$. For example, the large growth of $R_{g}$ predicted by the HKN parametrization at $x \geq 10^{-1}$ shown in Fig. 5.29 implies the steep behavior of $R_{C}$ at $x \geq 10^{-2}$ observed in Fig. [5.30. Consequently, by measuring $F_{2}^{c}$ it is also possible to constrain the existence and magnitude of the antishadowing effects.

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## DIS in the high-energy limit at next-to-leading order

## Giovanni A. Chirilli

Nowadays,it is widely accepted that non-linear dynamics effects dominate deep inelastic lepton hadrons scattering processes (DIS) at very high-energy (Regge limit), and non-linear equations have been derived in order to describe the evolution of the structure of hadronic matter at this regime. One of these equations is the Balitsky-Kovchegov equation (BK) derived by Balitsky [770] in the Wilson lines formalism, and by Kovchegov [741, 747] in the dipole frame. The Wilson line formalism is an operator language based on the concept of factorization of the scattering amplitude in rapidity space and on the extension of the application of the Operator Product Expansion (OPE) formalism to high-energy (Regge limit). So far, the OPE formalism was known only in the Bjorken limit as an expansion in terms of local operators or in terms of light ray operators.

The relevance of the BK equation for future experiments at an Electron Ion Collider (EIC) or Large electron Hadron Collider (LeHC) can be determined by the running of the coupling constant and the evolution kernel at the next-to-leading-order (NLO) approximation (NLO corrections in power of the strong coupling constant $\alpha_{s}$ ). The argument of the coupling constant has been obtained by the authors of ref. [833, 834] where only the quark contribution has been calculated explicitly, while the gluonic part was obtained conjecturing that its contribution would follow the same pattern of the quark contribution. However, this result did not fully solve the problem of the argument of the running coupling constant due to an ambiguity of one term which is not proportional to $b=\frac{11}{3} N_{c}-\frac{2}{3} n_{f}$. The complete results of the NLO-BK kernel including the gluon contribution to the argument of the coupling constant has been obtained in [835] where it was shown that the result agrees with
the NLO Balitsky-Fadin-Kuraev-Lipatov (BFKL) kernel. The BFKL equation [836, 60] can be obtained from the BK equation by dropping out the non linear terms. Indeed, a caveat of such a linear evolution equation is the violation at very high energy of the unitarity condition which is instead preserved by the BK equation.

Conformal symmetry is a symmetry violated in QCD by the running of the coupling constant. What one would then expect from the calculation of the NLO BK-kernel is that the only source of violation of such symmetry come from the running of coupling while the rest of the kernel preserves conformal (Möbius) symmetry. However, although Wilson lines are formally conformal invariant, at one loop correction they are rapidity-divergent, and since it is not known how to regulate them in a conformally invariant way, the NLOBK kernel contains non-conformal terms (besides to the running coupling constant) as a remnant of the prescription used to cure such divergences. In order to study the source of the loss of conformal invariance, it is convenient to consider a conformally invariant theory like the $\mathcal{N}=4$ super-symmetric Yang-Mills (SYM) theory. The NLO evolution kernel obtained in this framework is also not conformally invariant 837, contrary to what one would expect from a conformal field theory. It was then shown in [837, that suitable operators for the description of processes at high-energy (Regge) theory are composite conformal (Wilson line) operators constructed order by order in perturbation theory. These operators absorb the undesired non conformal terms in the same way as counterterms are added to renormalize local composite operators in order to restore the symmetry that the bare operator lost at the level of NLO (and higher) corrections. Indeed, the NLO evolution of such composite conformal operators in QCD resolve in a running coupling part and in a conformally invariant part. In ref. [837, 838], the conformal expression for the NLO BFKL has been obtained for the first time.

In order to obtain the full NLO amplitude for DIS at high energy, one needs to calculate the coefficient function (photon impact factor) at NLO and convolute it with the NLO evolution kernel of the relative operator (the NLO BK kernel). The NLO impact factor has been calculated in ref. [839] where an analytic expression (in coordinate space) has been obtained for the first time.

High-energy operator product expansion: In the usual OPE, due to the presence of two different scales of the transverse momentum $k_{\perp}$, one introduces a factorization scale, usually denoted by $\mu$, which factorizes the amplitude of DIS processes in pertubatively calculable contributions (hard part) and in a non-pertubatively calculable ones (soft part) represented by matrix elements made of light-ray operators. The evolution of such matrix elements with respect to the renormalization point $\mu$ is the DGLAP evolution equation.

At high-energy (Regge limit), all the transverse momenta are of the same order of magnitude. Therefore, a suitable factorization scale would be the rapidity scale: one introduces rapidity $(\eta)$ which separates "fast" fields from "slow" fields. Thus, the amplitude of the process can be represented as a convolution of contributions coming from fields with rapidity $\eta<Y$ (fast fields) and contributions coming from fields with rapidity $\eta>Y$ (slow fields). As in the case of the usual OPE, the integration over the fields with rapidity $\eta<Y$ gives us the coefficient functions while the integrations over fields with rapidity $\eta>Y$ are the matrix elements of the operators. A general feature of high-energy scattering is that a fast particle moves along its straight-line classical trajectory and the only quantum effect is the eikonal phase factor acquired along this propagation path. In QCD, for the fast quark or gluon scattering off some target, this eikonal phase factor is a Wilson line - an infinite
gauge link ordered along the straight line collinear to the particle's velocity $n^{\mu}$ :

$$
\begin{equation*}
U^{\eta}\left(x_{\perp}\right)=\operatorname{Pexp}\left\{i g \int_{-\infty}^{\infty} d u n_{\mu} A^{\mu}\left(u n+x_{\perp}\right)\right\} \tag{5.44}
\end{equation*}
$$

Here, $A_{\mu}$ is the gluon field of the target, $x_{\perp}$ is the transverse position of the particle which remains unchanged throughout the collision, and the index $\eta$ labels the rapidity of the particle. Repeating the above argument for the target (moving fast in the spectator's frame) we see that particles with very different rapidities perceive each other as Wilson lines and therefore Wilson-line operators are the convenient effective degrees of freedom in high-energy QCD (for a review, see Ref. [840]). The expansion of the T product of two electromagnetic currents at high-energy (Regge limit) is then in terms of Wilson lines

$$
\begin{aligned}
& T\left\{\hat{j}_{\mu}(x) \hat{j}_{\nu}(y)\right\}=\int d^{2} z_{1} d^{2} z_{2} I_{\mu \nu}^{\mathrm{LO}}\left(x, y ; z_{1}, z_{2}\right) \hat{\mathcal{U}}\left(z_{1}, z_{2}\right) \\
& +\int d^{2} z_{1} d^{2} z_{2} d^{2} z_{3} I_{\mu \nu}^{\mathrm{NLO}}\left(x, y ; z_{1}, z_{2}, z_{3}\right)\left[\hat{\mathcal{U}}\left(z_{1}, z_{3}\right)+\hat{\mathcal{U}}\left(z_{2}, z_{3}\right)-\hat{\mathcal{U}}\left(z_{1}, z_{2}\right)-\hat{\mathcal{U}}\left(z_{1}, z_{3}\right) \hat{\mathcal{U}}\left(z_{3}, z_{2}\right)\right]
\end{aligned}
$$

where

$$
\begin{equation*}
\hat{\mathcal{U}}^{\eta}\left(x_{\perp}, y_{\perp}\right)=1-\frac{1}{N_{c}} \operatorname{Tr}\left\{\hat{U}^{\eta}\left(x_{\perp}\right) \hat{U}^{\dagger \eta}\left(y_{\perp}\right)\right\} \tag{5.45}
\end{equation*}
$$

The evolution of the Wilson line operator in eq. (5.45) is given by the BK equation [770, 741, 747,

$$
\begin{array}{r}
\frac{d}{d \eta} \hat{\mathcal{U}}(x, y)=\frac{\alpha_{s} N_{c}}{2 \pi^{2}} \int d^{2} z \frac{(x-y)^{2}}{(x-z)^{2}(z-y)^{2}}[\hat{\mathcal{U}}(x, z)+\hat{\mathcal{U}}(y, z) \\
-\hat{\mathcal{U}}(x, y)-\hat{\mathcal{U}}(x, z) \hat{\mathcal{U}}(z, y)] \tag{5.46}
\end{array}
$$

The first three terms correspond to the linear BFKL evolution equation [836, 60] and describe parton emission while the last term is responsible for parton annihilation. For sufficiently low $x_{B}$, parton emission balances parton annihilation so the partons reach the state of saturation [742, 841, 842] with the characteristic transverse momentum $Q_{s}$ growing with energy $1 / x_{B}$. The NLO evolution equation for composite Wilson line operator (preserving conformal invariance as explained in the introduction) has been calculated in [835, where one can find the full analytic expression.

In order to obtain the DIS amplitude at high-energy at the NLO, we now need the coefficient function ("impact factor") at next to leading order. Here, we present the NLO impact factor for the study of DIS in the linearized case (two gluon approximation) where the NLO BK equation reduces to the NLO BFKL equation. In this case the OPE at high energy for DIS reduces to

$$
\begin{align*}
& \frac{1}{N_{c}}(x-y)^{4} T\left\{\overline{\hat{\psi}}(x) \gamma^{\mu} \hat{\psi}(x) \overline{\hat{\psi}}(y) \gamma^{\nu} \hat{\psi}(y)\right\}  \tag{5.47}\\
& =\frac{\partial \kappa^{\alpha}}{\partial x^{\mu}} \frac{\partial \kappa^{\beta}}{\partial y^{\nu}} \int \frac{d z_{1} d z_{2}}{z_{12}^{4}} \hat{\mathcal{U}}_{a_{0}}\left(z_{1}, z_{2}\right)\left[\mathcal{I}_{\alpha \beta}^{\mathrm{LO}}\left(1+\frac{\alpha_{s}}{\pi}\right)+\mathcal{I}_{\alpha \beta}^{\mathrm{NLO}}\right]
\end{align*}
$$

where

$$
\begin{equation*}
\mathcal{I}_{\mathrm{LO}}^{\alpha \beta}\left(x, y ; z_{1}, z_{2}\right)=\mathcal{R}^{2} \frac{g^{\alpha \beta}\left(\zeta_{1} \cdot \zeta_{2}\right)-\zeta_{1}^{\alpha} \zeta_{2}^{\beta}-\zeta_{2}^{\alpha} \zeta_{1}^{\beta}}{\pi^{6}\left(\kappa \cdot \zeta_{1}\right)\left(\kappa \cdot \zeta_{2}\right)} \tag{5.48}
\end{equation*}
$$

is the LO impact factor and where we used the notation $\mathcal{R} \equiv \frac{\kappa^{2}\left(\zeta_{1} \cdot \zeta_{2}\right)}{2\left(\kappa \cdot \zeta_{1}\right)\left(\kappa \cdot \zeta_{2}\right)}$, and the conformal vectors $\kappa=\frac{\sqrt{s}}{2 x_{*}}\left(\frac{p_{1}}{s}-x^{2} p_{2}+x_{\perp}\right)-\frac{\sqrt{s}}{2 y_{*}}\left(\frac{p_{1}}{s}-y^{2} p_{2}+y_{\perp}\right), \zeta_{i}=\left(\frac{p_{1}}{s}+z_{i \perp}^{2} p_{2}+z_{i \perp}\right)$ with $x_{*}=p_{2}^{\mu} x_{\mu}=\frac{\sqrt{2}}{s} x^{+}$(s is the Mandelstam variable). The analytic expression of the NLO impact factor for DIS at high energies can be found in Ref. [839]. Note that the NLO impact factor is conformally (Möbius) invariant and is given by a linear combination of five conformal tensor structures as predicted in [843]. The next natural step would be the Fourier transformation of the result in ref. [839] (the NLO impact factor), which gives the momentum-space impact factor convenient for phenomenological applications (and available at present only as a combination of numerical and analytical expressions [844, 845, 846]).

Conclusions: We have briefly summarized the status of the NLO calculation of the structure function for DIS at high energy. The main ingredients for the full amplitude, namely the NLO BK kernel and the NLO IF, have been calculated. The main result of this analysis is that the OPE for high energy (Regge limit) is at the same status as the usual OPE in the Bjorken limit. This means that the factorization in rapidity did not break down at NLO accuracy. As an application of the factorization in rapidity, the full NLO analytic amplitude in $\mathcal{N}=4$ SYM was calculated, the NLO result for the Pomeron intercept at small $\alpha_{s}$ was confirmed, and for the first time the NLO Pomeron residue was obtained [847].

The Wilson line formalism proved to be very successful, not only in obtaining in a more efficient way many results that in the usual pertubative QCD mechanism ( pQCD ), were obtained after many years of calculations by several groups, but also to obtain some results that have not been obtained (not for lack of efforts) in the usual pQCD mechanism, like the NLO impact factor, the NLO conformal BFKL kernel and the NLO pomeron residue, and in addition to generalize these results to include the non linear effects dominant at high energies. Another example which proves the efficiency of this formalism is the calculation, in a very easy way, of the triple pomeron vertex for diffractive and non-diffractive ("fan diagrams") processes, including the subleading $N_{c}$ contributions 848.

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## Running Coupling in Small-x Physics

## Yuri V. Kovchegov

Running coupling corrections have been included into BFKL/BK/JIMWLK evolution following the Brodsky-Lepage-Mackenzie (BLM) scale-setting procedure 849] in 850, 834, 833, 851, 751. The BLM prescription requires one to first re-sum the contribution of all quark bubble corrections giving powers of $\alpha_{\mu} N_{f}$, with $N_{f}$ the number of quark flavors and $\alpha_{\mu}$ the physical coupling at some arbitrary renormalization scale $\mu$. One then has to complete $N_{f}$ to the full beta-function by replacing $N_{f} \rightarrow-6 \pi \beta_{2}$ in the obtained expression. Here, $\beta_{2}=\left(11 N_{c}-2 N_{f}\right) /(12 \pi)$ is the one-loop QCD beta-function. After this, the powers of $\alpha_{\mu} \beta_{2}$ should combine into physical running couplings $\alpha_{s}\left(Q^{2}\right)=\alpha_{\mu} /\left(1+\alpha_{\mu} \beta_{2} \ln \left(Q^{2} / \mu^{2}\right)\right)$ at various momentum scales $Q$ which would follow from this calculation. The running coupling below will be written in the $\overline{\mathrm{M} S}$ renormalization scheme.

Below we will concentrate on the case of running coupling corrections to the BFKL and BK evolution equations. Running-coupling corrections to the JIMWLK equation can
be found in [834, 751]. At the moment the running coupling corrections to BK have been better explored numerically than those for JIMWLK.

Analytic result: Let us briefly summarize the results of [834, 833, 751]. The BalitskyKovchegov evolution equation with the running coupling corrections included (rcBK) reads

$$
\begin{equation*}
\frac{\partial S\left(\underline{x}_{0}, \underline{x}_{1} ; Y\right)}{\partial Y}=\mathcal{R}[S]-\mathcal{S}[S] . \tag{5.49}
\end{equation*}
$$

Here we use the $S$-matrix notation, related to the forward dipole amplitude by $S\left(\underline{x}_{0}, \underline{x}_{1} ; Y\right)=$ $1-N\left(\underline{x}_{0}, \underline{x}_{1} ; Y\right)$. The first term on the right hand side of Eq. (5.49) is referred to as the running coupling contribution, while the second term on the right hand side of Eq. (5.49) is referred to as the subtraction contribution. Separation into the two parts is arbitrary, and was done differently in 833 ] and [834, with the net sum being the same [751].

The running coupling part was calculated independently in 833] and in [834: the results of those calculations are

$$
\begin{align*}
\mathcal{R}^{\mathrm{Bal}}[S] & =\int d^{2} z \tilde{K}^{\mathrm{Bal}}\left(\underline{x}_{0}, \underline{x}_{1}, \underline{z}\right)\left[S\left(\underline{x}_{0}, \underline{z} ; Y\right) S\left(\underline{z}, \underline{x}_{1} ; Y\right)-S\left(\underline{x}_{0}, \underline{x}_{1} ; Y\right)\right]  \tag{5.50}\\
\mathcal{R}^{\mathrm{KW}}[S] & =\int d^{2} z \tilde{K}^{\mathrm{KW}}\left(\underline{x}_{0}, \underline{x}_{1}, \underline{z}\right)\left[S\left(\underline{x}_{0}, \underline{z} ; Y\right) S\left(\underline{z}, \underline{x}_{1} ; Y\right)-S\left(\underline{x}_{0}, \underline{x}_{1} ; Y\right)\right] . \tag{5.51}
\end{align*}
$$

The integral kernels in the two cases are given by

$$
\begin{equation*}
\tilde{K}^{\mathrm{Bal}}\left(\underline{r}, \underline{r}_{1}, \underline{r}_{2}\right)=\frac{N_{c} \alpha_{s}\left(r^{2}\right)}{2 \pi^{2}}\left[\frac{r^{2}}{r_{1}^{2} r_{2}^{2}}+\frac{1}{r_{1}^{2}}\left(\frac{\alpha_{s}\left(r_{1}^{2}\right)}{\alpha_{s}\left(r_{2}^{2}\right)}-1\right)+\frac{1}{r_{2}^{2}}\left(\frac{\alpha_{s}\left(r_{2}^{2}\right)}{\alpha_{s}\left(r_{1}^{2}\right)}-1\right)\right] \tag{5.52}
\end{equation*}
$$

as found in 833 and by

$$
\begin{equation*}
\tilde{K}^{\mathrm{KW}}\left(\underline{r}, \underline{r}_{1}, \underline{r}_{2}\right)=\frac{N_{c}}{2 \pi^{2}}\left[\alpha_{s}\left(r_{1}^{2}\right) \frac{1}{r_{1}^{2}}-2 \frac{\alpha_{s}\left(r_{1}^{2}\right) \alpha_{s}\left(r_{2}^{2}\right)}{\alpha_{s}\left(R^{2}\right)} \frac{r_{1} \cdot \underline{r}_{2}}{r_{1}^{2} r_{2}^{2}}+\alpha_{s}\left(r_{2}^{2}\right) \frac{1}{r_{2}^{2}}\right] \tag{5.53}
\end{equation*}
$$

as found in [834], where

$$
\begin{equation*}
R^{2}\left(\underline{r}, \underline{r}_{1}, \underline{r}_{2}\right)=r_{1} r_{2}\left(\frac{r_{2}}{r_{1}}\right)^{\frac{r_{1}^{2}+r_{2}^{2}}{r_{1}^{2}-r_{2}^{2}}-2 \frac{r_{1}^{2} r_{2}^{2}}{r_{1}-r_{2}} \frac{1}{r_{1}^{2}-r_{2}^{2}}} . \tag{5.54}
\end{equation*}
$$

One notices immediately that $\mathcal{R}^{\mathrm{Bal}}[S]$ calculated in [833] is different from $\mathcal{R}^{\mathrm{KW}}[S]$ calculated in 834 due to the difference in the kernels $\tilde{K}^{\text {Bal }}$ and $\tilde{K}^{\mathrm{KW}}$ in Eqs. (5.52) and (5.53). However that does not imply disagreement between the calculations of 833] and [834): after all, it is the full kernel on the right of Eq. (5.49), $\mathcal{R}[S]-\mathcal{S}[S]$, that needs to be compared. To do that, one has to calculate the second term on the right hand side of Eq. (5.49) (the subtraction contribution). This was done in [751, yielding

$$
\begin{align*}
\mathcal{S}[S]= & \alpha_{\mu}^{2} \int d^{2} z_{1} d^{2} z_{2} K_{(1)}\left(\underline{x}_{0}, \underline{x}_{1} ; \underline{z}_{1}, \underline{z}_{2}\right) \\
& \times\left[S\left(\underline{x}_{0}, \underline{w}, Y\right) S\left(\underline{w}, \underline{x}_{1}, Y\right)-S\left(\underline{x}_{0}, \underline{z}_{1}, Y\right) S\left(\underline{z}_{2}, \underline{x}_{1}, Y\right)\right] \tag{5.55}
\end{align*}
$$

and the re-summed BK kernel $K_{(1)}$ can be found in the original reference. Substituting $\underline{w}=\underline{z}_{1}$ (or, equivalently, $\underline{w}=\underline{z}_{2}$ ) in Eq. (55.55) yields the subtraction term $\mathcal{S}^{\text {Bal }}[S]$, which has to be subtracted from $\mathcal{R}^{\mathrm{Bal}}[S]$ calculated in [833] and given by Eq. (55.50) to obtain


Figure 5.31. Solutions of the complete (all orders in $\alpha_{s} \beta_{2}$ ) evolution equation given in Eq. (5.49) (solid lines), and of the equation with Balitsky's (dashed lines) and KW's (dashed-dotted) running coupling schemes at rapidities $Y=0,3$ and 10. Left plot uses quasi-classical McLerran-Venugopalan (MV) initial condition. The right plot employs the initial condition given by the dipole amplitude at rapidity $Y=35$ evolved using Balitsky's running coupling scheme and with $r$-dependence rescaled down such that $Q_{s}=Q_{s}^{\prime}=1 \mathrm{GeV}$.
the complete evolution equation re-summing all orders of $\alpha_{s} N_{f}$ in the kernel. Substituting $\underline{w}=\underline{z}=\alpha \underline{z}_{1}+(1-\alpha) \underline{z}_{2}$ in Eq. (5.55) yields the term $\mathcal{S}^{\mathrm{KW}}[S]$, which has to be subtracted from $\mathcal{R}^{\mathrm{KW}}[S]$ calculated in 834 and given in Eq. (5.51) again to obtain the complete evolution equation re-summing all orders of $\alpha_{s} N_{f}$ in the kernel.

Numerical Solution: The numerical solution of the running-coupling BK (rcBK) evolution just presented was performed in [751] and plotted in Fig. 5.31. One plots the runningcoupling parts from Eqs. (5.50) and (5.51) [834, 833] (dashed and dash-dotted lines correspondingly), along with the full solution (solid line). As one can see the full solution is best approximated by the Balitsky's running coupling scheme from Eq. (5.50) 833. Hence in most phenomenological applications one simply solves rcBK with Balitsky's prescription [85), 852]. Note that the rcBK solution also exhibits the property of geometric scaling [752], as was shown in [751.

Running-coupling BFKL evolution: The running-coupling BFKL equation (rcBFKL) was constructed in 851 and reads

$$
\begin{align*}
\frac{\partial \phi(k, Y)}{\partial Y}=\frac{N_{c}}{2 \pi^{2}} \int d^{2} q\{ & \frac{2}{(\boldsymbol{k}-\boldsymbol{q})^{2}} \alpha_{s}\left((\boldsymbol{k}-\boldsymbol{q})^{2} e^{-5 / 3}\right) \phi(q, Y) \\
& \left.-\frac{\boldsymbol{k}^{2}}{\boldsymbol{q}^{2}(\boldsymbol{k}-\boldsymbol{q})^{2}} \frac{\alpha_{s}\left(\boldsymbol{q}^{2} e^{-5 / 3}\right) \alpha_{s}\left((\boldsymbol{k}-\boldsymbol{q})^{2} e^{-5 / 3}\right)}{\alpha_{s}\left(\boldsymbol{k}^{2} e^{-5 / 3}\right)} \phi(k, Y)\right\}, \tag{5.56}
\end{align*}
$$

where the unintegrated gluon distribution $\phi(k, Y)$ is defined by

$$
\begin{equation*}
N\left(x_{01}, Y\right)=\int \frac{d^{2} k}{(2 \pi)^{2}}\left(1-e^{i \boldsymbol{k} \cdot \boldsymbol{x}_{01}}\right) \tilde{N}(k, Y) \tag{5.57}
\end{equation*}
$$

with

$$
\begin{equation*}
\alpha_{s}\left(k^{2}\right) \phi(k, Y)=\frac{N_{c} S_{\perp}}{(2 \pi)^{3}} k^{2} \tilde{N}(k, Y) . \tag{5.58}
\end{equation*}
$$

Here $S_{\perp}$ is the transverse area of the target. The running-coupling BFKL equation (5.56) was originally conjectured in [853, 854] by postulating the validity of the bootstrap equation for running-coupling corrections.

## Running-coupling and higher-order effects on the saturation scale

Guillaume Beuf

The DGLAP [855, 856, 857] and BFKL [858, 59, 60] equations give the evolution with kinematics of the partonic content of hadrons and nuclei in the regime where these are dilute. As these equations are linear, they can be solved analytically by using a Mellin tranform. By contrast, when the phenomenon of gluon saturation [742] is taken taken into account, the relevant evolution equations - B-JIMWLK [770, 756, 757, 759, 760, 761, 745, 762, 763] or BK [770, 741, 747] - are nonlinear, and thus cannot be solved analytically.

Nevertheless, the solutions of these nonlinear equations in the leading order (LO) approximation (where the coupling $\alpha_{s}$ is kept fixed) are well understood, by combining results from numerical simulations [859, 750,860 and analytical asymptotic expansions [755, 861, 862, 863, 864. Indeed, the BK equation belongs to a well-studied class of nonlinear equations, whose solutions develop asymptotically a universal traveling wave-front structure [865, 866], which is independent of the initial condition 3 . In the context of QCD, that traveling wavefront structure of the solution implies the geometric scaling [752] property found in the DIS data at HERA: the total virtual photon - target cross sections $\sigma_{T, L}^{\gamma^{*}}\left(Y, Q^{2}\right)$ depend on $Y$ and $Q^{2}$ essentially only through the combination $Q^{2} / Q_{s}^{2}(Y)$, because the dipole-target amplitude solution of the BK equation depends only on $r^{2} Q_{s}^{2}(Y)$ at large $Y, r$ being the dipole size. The evolution of the saturation scale $Q_{s}^{2}(Y)$ is obtained from the propagation of the wave-front. For the LO BK equation, one gets a large $Y$ expansion of the form

$$
\begin{equation*}
\log Q_{s}^{2}(Y)=a_{1} Y+a_{0} \log Y+\text { Const. }+a_{-1 / 2} Y^{-1 / 2}+\mathcal{O}\left(Y^{-1}\right) \tag{5.59}
\end{equation*}
$$

where $a_{1}, a_{0}$ and $a_{-1 / 2}$ are three known universal coefficients [864], whereas the constant term and all the ones of order $Y^{-1}$ or less do depend on the initial conditions, i.e. on the nature of the target used for the DIS. From geometric considerations, the initial $Q_{s}^{2}$ of a nucleus $A$ is enhanced by a factor $A^{1 / 3}$ with respect to that of a proton. That nuclear enhancement of $Q_{s}^{2}(Y)$ is preserved by the LO high-energy evolution, in the constant term of the expansion (5.59). Both from numerical simulations and from the expansion (5.59), one learns that the evolution of $Q_{s}^{2}(Y)$ implied by the LO BK equation is too fast to be compatible with the data for DIS and other observables, which favor $\log Q_{s}^{2}(Y) \sim \lambda Y$, with $\lambda \simeq 0.2$ or 0.3 . We are thus forced to consider higher order corrections to the BK equation.

Running vs. fixed coupling: As discussed in this section by Chirilli, the BK equation is now known at next-to-leading order (NLO) [835, 837]. However, its solutions are much less understood than the ones of the LO equation. Indeed no numerical simulations of the full NLO BK equation have been performed yet, for technical reasons, but only simulations [859, 750, 860, 751, 867 of the BK equation with LO kernel and running coupling $\alpha_{s}$, with various prescriptions used to set the scale in the coupling. By contrast, it is non-trivial to go from fixed coupling to running coupling in the analytical studies, since it leads to a different class

[^277]of wave-front solutions, for which universality of the asymptotics is not fully established. The inclusion of other NLO corrections gives however no additional difficulty. Let us first discuss the effects of running coupling only.

A priori, the running of the coupling brings the additional scale $\Lambda_{Q C D}$ into the problem, which may spoil the geometric scaling property. Indeed, there is no interval where the solutions of the running coupling BK equation show exact geometric scaling, by contrast to fixed coupling solutions, but they satisfy an approximate geometric scaling in some range. Equivalently, the wave-front in the solutions is being slowly distorted during its propagation, instead of being uniformly translated as in the fixed coupling case.

Running coupling effects turn the asymptotic behavior of the saturation scale into $\log Q_{s}^{2}(Y) \propto \sqrt{Y}$, as found in early analytical studies [742, 755, 861, 863. More precisely its large $Y$ asymptotics writes

$$
\begin{equation*}
\log \left(Q_{s}^{2}(Y) / \Lambda_{Q C D}^{2}\right)=b_{1 / 2} \sqrt{Y}+b_{1 / 6} Y^{1 / 6}+b_{0}+b_{-1 / 6} Y^{-1 / 6}+b_{-1 / 3} Y^{-1 / 3}+\mathcal{O}\left(Y^{-1 / 2}\right) \tag{5.60}
\end{equation*}
$$

where the first five terms are universal and known 4 , whereas the following ones of order $Y^{-1 / 2}$ or less are sensitive to the initial conditions. The universality of the constant term $b_{0}$ in (5.60) implies that initial conditions effects such as the nuclear $A^{1 / 3}$ enhancement of $Q_{s}^{2}$ are washed-out at high rapidity when the coupling is running, as first predicted in [869]. Numerically, it has been found [750, 860, 870] that this effect happens at very high rapidity. Hence, the nuclear enhancement of $Q_{s}^{2}$, which is one of the motivations for doing nuclear DIS at the EIC, should still be present in the kinematical range accessible at the EIC. Remarkably, the evolution of the saturation scale in the running coupling case is such that very good fits of DIS data can be performed with solutions of the running coupling BK equation [85, 820], by contrast to the fixed coupling case, without the inclusion of other NLO effects.

Other NLO effects: Apart from the contributions re-summed into the running of the coupling, there are large NLO corrections to the BK kernel, related to the large NLO corrections to the BFKL kernel [722, 723].

In a conformal gauge field theory, terms of arbitrary $\mathrm{N}^{n} \mathrm{LO}$ order from the kernel would contribute at each order of the expansion (5.59). By contrast, the running of the coupling is dynamically quenching the effect on the solutions of higher order terms in the kernel. NLO contributions start to appear at order $Y^{0}$ in (5.60), NNLO contributions at order $Y^{-1 / 2}$ and so on. Moreover, the coefficient $b_{-1 / 6}$ has been found to be NLO-independent [868]. Apart from the running of the coupling, NLO contributions thus affect mostly the normalization of $Q_{s}^{2}(Y)$ at large $Y$, via $b_{0}$, and only mildly the asymptotic $Y$-evolution of $Q_{s}^{2}(Y)$, via $b_{-1 / 3} Y^{-1 / 3}$ and further subleading terms. That property is indeed seen in numerical simulations with running coupling and a subset of other NLO contributions included 867. That result shed some light on the spectacular success of the running coupling LO BK equation to describe DIS data. There is a degeneracy in (5.60) between the contribution of $\Lambda_{Q C D}$ and $b_{0}$ to $Q_{s}^{2}(Y)$. Hence, treating $\Lambda_{Q C D}$ as a free fit parameter as in Refs. 85, 820] allows one to fit the bulk of NLO effects, without actually simulating the BK evolution with NLO kernel.

Several prescriptions [833, 834] have been proposed to split NLO corrections into contributions to the running coupling or to the kernel. Hence, BK equations with running

[^278]coupling and LO kernel obtained following different prescriptions differ formally by terms of order NLO and beyond in the kernel. In numerical simulations of such running coupling LO BK equations [751], solutions with different prescriptions differ at large $Y$ mostly by a constant rescaling of $Q_{s}^{2}(Y)$, in agreement with our previous discussion.

The problems brought by the impact-parameter dependence: Implicitly, we have discussed so far only results from studies of impact parameter independent solutions of the BK equation. The BK equation preserves unitarity at fixed impact parameter. However, its impact parameter dependent solutions violate unitarity since they violate the Froissart bound [871] on the cross-section [872, 867], due to the unphysical possibility of gluon emission at arbitrarily long range in the transverse plane. The running of the coupling reveals another problem: there is a reappearance of the diffusion into the infrared [867, which was thought to be cured by gluon saturation, from studies of impact parameter independent solutions of the BK equation. Hence, the impact parameter dependent solutions of the BK solutions are very sensitive to strongly coupled infrared physics, which is not yet implemented in the formalism. This is the most challenging open theoretical problem with regard to gluon saturation. Therefore, it is not yet clear to what extent the results about impact parameter independent solutions presented in the previous sections are reliable for realistic proton or nuclear targets.

### 5.4 Diffractive DIS ( $\mathbf{F}_{2}^{D}, \mathbf{F}_{L}^{D}$, charm contribution)

## Diffraction in $e+p$ and $e+A$ collisions

Cyrille Marquet

A non-negligible fraction of the events in DIS are diffractive, meaning that the hadronic target, of mass $M$, escapes the collision intact. As a colorless object has been exchanged in the t-channel, there is rapidity gap void of particles in the final state, between the outgoing target and the diffractive final state $X$, made up of all the other particles in the event. On top of $x$ and $Q^{2}$, two additional kinematic invariants are needed to characterize diffraction in DIS: the momentum transfer $t<0$ at the hadronic vertex, and the mass $M_{X}$ of the diffractive final state. In practice, the variable $M_{X}$ is sometimes traded for $\beta$ and the variable $x$ is traded for $x_{\mathbb{P}}$-these are defined as

$$
\begin{equation*}
\beta=\frac{Q^{2}}{Q^{2}+M_{X}^{2}-t} ; x_{\mathbb{P}}=\frac{x}{\beta}=\frac{Q^{2}+M_{X}^{2}-t}{Q^{2}+W^{2}-M^{2}} . \tag{5.61}
\end{equation*}
$$

Small values of $\beta$ refer to events with diffractive masses much bigger than the photon virtuality, while values of $\beta$ close to unity refer to the opposite situation. $x_{\mathbb{P}}$ is useful because it characterizes the size of the rapidity gap $\Delta \eta \simeq \ln \left(1 / x_{\mathbb{P}}\right)$.

There are events in which the hadronic target, instead of staying intact, may dissociate into a low-mass excited state Y, while still leaving a rapidity gap in the final state. These events are also classified as diffractive, they occur only if the mass $M_{Y}$ of the excited state is close enough to the initial mass $M$. Coherent diffraction is employed when the target scatters elastically ( $\mathrm{ep} \rightarrow \mathrm{eXp}$ ), while incoherent diffraction refers to the more general case $e p \rightarrow e X Y$ which is a sum of coherent diffraction $(Y=p)$ and target-dissociative diffraction $(\mathrm{Y} \neq \mathrm{p})$. The former dominates at low $|t|$ and the latter at large $|t|$.

While in the leading-twist approximation of QCD there is a collinear factorization theorem to compute diffractive structure functions in DIS at large $Q^{2}$, the description of hard diffraction in this framework is not as natural as for inclusive events. This is reflected in the fact that standard parton distribution functions (pdfs) are of no help to compute $F_{2}^{D}$, and one has to introduce a different set of parton distributions called diffractive pdfs (dpdfs). Therefore in the collinear factorization framework, the description of the parton content of the proton depends on whether or not the final state is diffractive. While this is successful - and should be since collinear factorization is a good approximation of QCD at large $Q^{2}$ - conceptually it is not so satisfactory as one would like to be able to describe any process with a single proton wave function.

No further conceptual advances are expected within the leading-twist approximation of QCD. There are some technical improvements that can be made, for instance it is nowadays practically impossible to extract dpdfs without assuming what is called Regge factorization: $\operatorname{dpdf}\left(x_{\mathbb{P}}, t, \beta, Q^{2}\right)=f\left(x_{\mathbb{P}}, t\right) g\left(\beta, Q^{2}\right)$. This is not satisfactory, since such a factorization is not a property of QCD. However, there is little doubt that if one could bypass this practical problem - perhaps with a larger data sample in all four directions: $Q^{2}, \beta, x_{\mathbb{P}}$ and $t$ - this approach would succeed at large $Q^{2}$.

But in fact, the purpose of an electron-ion collider is not to check whether DGLAP evolution will work at large $Q^{2}$, the goal is rather to explore what we don't know as well: the non-linear regime of QCD where collinear factorization breaks down. To be more specific, we are interested in the regime $Q^{2}<5 \mathrm{GeV}^{2}$ and $x$ as small as possible. Interestingly enough, studying the non-linear saturation regime will be easier with diffractive than with inclusive
measurements. This is so because at small $x$, diffractive processes are mostly sensitive to quantum fluctuations in the proton wave function that have a virtuality of order $Q_{s}^{2}$, instead of $Q^{2}$. As a result, power corrections (not the generic $\Lambda_{Q C D}^{2} / Q^{2}$ corrections, but rather the sub-class of them of order $Q_{s}^{2} / Q^{2}$ important at small $x$ ) are expected to come into play starting from a higher value of $Q^{2}$ in diffractive DIS, compared to inclusive DIS. In fact, there is already a hint that this is happening at HERA: collinear factorization starts to fail below about $2 \mathrm{GeV}^{2}$ in the case of $F_{2}$, while already below about $8 \mathrm{GeV}^{2}$ in the case of $F_{2}^{D}$.

The QCD description of diffractive DIS in the small- $x$ limit turns out to be much more insightful than that of the large- $Q^{2}$ limit. It is so because at small $x$, DDIS can be expressed in the Good-Walker picture (which was originally imagined for soft diffraction in hadronhadron collisions), with the benefit that, thanks to the point-like nature of the photon, the modeling part of the Good-Walker approach can be replaced by actual QCD computations. This remarkable realization of the Good-Walker picture in small-x DIS is more commonly referred to as the dipole picture: dipoles are eigenstates of high-energy scattering in QCD, and it is known how to expand the photon wave function onto the dipole basis. At the end in this approach, the parton content of the proton - both in the linear and non-linear regimes - is parametrized through the dipole cross section. As a result, diffractive structure functions also feature geometric scaling [873]. Another important fact is that at small $x$, diffraction can be entirely predicted, once the dipole cross section has been constrained with inclusive data.

In spite of the fact that this approach has been able to successfully predict $F_{2}^{D}$ at small $x$, there is still important conceptual progress to be made. For instance, the transverse impact parameter dependence of the dipole scattering amplitude is very poorly constrained. Indeed, one has been able to describe $F_{2}$ and correctly predict $F_{2}^{D}$ with two kinds of impact parameter dependences, neither of which is fully satisfactory. In a first class of dipole models, the impact parameter profile of the proton is independent of energy, yielding a dipole cross section bounded from above. In the other class of models, the black-disk regime of maximal scattering strength spreads too quickly in the transverse plane with increasing dipole size $r$, leading to a dipole cross section which diverges for large $r$. It is quite clear that the LHeC is needed to help us understand better this issue.

Finally, let us say a few important words on ep $\rightarrow$ eXY diffractive events. In past experiments, events with $Y \neq p$ have mostly been regarded as background, and model-dependent subtractions have been applied to data, yielding large normalization uncertainties. Within the kinematic reach of HERA, it has been observed that the ratio $d \sigma^{e p \rightarrow e X Y} / d \sigma^{e p \rightarrow e X p}$ is a constant independent of all kinematic variables other than $M_{Y}$ and $t$ (that ratio increases with $M_{Y}$ and $|t|$ ). Here we would like to emphazise that proton-dissociative events are also intrinsically interesting. For instance, at small $x$ the cross section difference $d \sigma^{e p \rightarrow e X Y}-d \sigma^{e p \rightarrow e X p}$ is $1 / N_{c}^{2}$ suppressed, meaning that if it were measured accurately, it would give access to details of the QCD dynamics which are untestable otherwise. The EIC provides such an opportunity.

After many fixed target experiments, it took a collider to discover diffractive events in $\mathrm{e}+\mathrm{p}$. Since no e+A collider has ever been built, diffraction in $\mathrm{e}+\mathrm{A}$ has simply never been measured. That such a deficiency exists in our knowledge of nuclear structure is compelling enough to build the EIC. Everything we would learn about DDIS off nuclei at the EIC will be new, in any kinematical domain, implying a huge discovery potential. Nevertheless, we have expectations of what diffraction off nuclei should look like, based on our current understanding of QCD. For instance, the theory of nuclear shadowing allows the
constuction of nuclear DPDFs for large $Q^{2}$ physics, while within the Color Glass Condensate framework, nuclear diffractive structure functions can be predicted at small $x$. Depending on these kinematics, different patterns of nuclear shadowing or antishadowing as a function of $\beta$ and $x_{\mathbb{P}}$ are expected. This is just one example out of many that should be checked with an e+A collider. Since the current predictions rely on rather simple models for impact parameter dependence, they need to be confronted to data, in order to, in return, improve our understanding.

Finally, there is one aspect of diffraction which is specific to nuclei that one should mention. The structure of incoherent diffraction $\mathrm{eA} \rightarrow \mathrm{eXY}$ is more complex than with a proton target, and also can teach us a lot more. In the case of a target nucleus, we expect the following qualitative changes in the $t$ dependence. First, the low- $|t|$ regime in which the nucleus scatters elastically will be dominant up to a smaller value of $|t|$ (to about $|t|=0.05 \mathrm{GeV}^{2}$ ) compared to the proton case, reflecting the larger size of the nucleus. Then, the nucleus-dissociative regime will comprise two parts: an intermediate regime in momentum transfer up to about $0.7 \mathrm{GeV}^{2}$ where the nucleus will predominantly break up into its constituents nucleons, and a large $-|t|$ regime where the nucleons inside the nucleus will also break up, implying pion production in the $Y$ system for instance. These are only qualitative expectations, it is crucial to study this aspect of diffraction quantitatively in order to complete our understanding of the structure of nuclei.

## Expectations for e+A from the CGC

## Cyrille Marquet

In this work, hard diffraction in electron-nucleus (e+A) collisions is considered within the IPsat model, 600 corresponding to the classical limit of the Color Glass Condensate approach. This effective theory of QCD at high partonic density is the most natural framework to describe the saturation phenomenon, and therefore to study e+A scattering at high energies, in particular diffractive observables. Here we shall focus on the nuclear diffractive structure function $F_{2, A}^{D}$.

Let us recall the kinematics of diffractive DIS: $\gamma^{*} A \rightarrow X A$. With a momentum transfer $t \leq 0$, the proton/nucleus gets out of the $\gamma^{*}-A$ collision intact, and is separated by a rapidity gap from the other final-state particles whose invariant mass we denote $M_{X}$. The photon virtuality is denoted $Q^{2}$, and the $\gamma^{*}-A$ total energy $W$. It is convenient to introduce the following variables: $x=Q^{2} /\left(Q^{2}+W^{2}\right), \beta=Q^{2} /\left(Q^{2}+M_{X}^{2}\right)$ and $x_{\mathbb{P}}=x / \beta$. The size of the rapidity gap is $\ln \left(1 / x_{\mathbb{P}}\right)$.

The diffractive structure function is expressed as a function of $\beta, x_{\mathbb{P}}, Q^{2}$, and $t$, and we will only consider the $t$-integrated structure function $F_{2}^{D, 3}$. While at large values of $x_{\mathbb{P}}$ and $Q^{2}$, the leading-twist collinear factorization is appropriate to describe hard diffraction off protons, this is not the case at small $x_{\mathbb{P}}$ or off nuclei, as higher twists are enhanced by $\sim\left(A / x_{\mathbb{P}}\right)^{0.3}$. In this situation, the dipole picture is better suited to address the problem. It naturally incorporates the description of both inclusive and diffractive events into a common theoretical framework: [781, 874, 875] the same dipole-nucleus scattering amplitudes, which can be computed treating the nucleus as a CGC, enter in the formulation of the inclusive and diffractive cross-sections.

Diffractive structure functions in the dipole picture: In our approach, $F_{2}^{D}=F_{T}^{q \bar{q}}+$ $F_{L}^{q \bar{q}}+F_{T}^{q \bar{q} g}$ where the different pieces correspond to transversely ( T ) or longitudinally ( L )
polarized photons dissociating into a $q \bar{q}$ or $q \bar{q} g$ final state. For instance, the $q \bar{q}$ contributions are
$x_{\mathbb{P}} F_{T}^{q \bar{q}}\left(\beta, x_{\mathbb{P}}, Q^{2}\right)=\frac{N_{c} Q^{4}}{8 \pi^{3} \beta} \sum_{f} e_{f}^{2} \int_{0}^{1} d z \Theta\left(\kappa_{f}^{2}\right) z(1-z)\left[f_{T}(z) \varepsilon_{f}^{2}(z) I_{1}\left(\kappa_{f}, \epsilon_{f}\right)+m_{f}^{2} I_{0}\left(\kappa_{f}, \epsilon_{f}\right)\right]$,
$x_{\mathbb{P}} F_{L}^{q \bar{q}}\left(\beta, x_{\mathbb{P}}, Q^{2}\right)=\frac{N_{c} Q^{6}}{8 \pi^{3} \beta} \sum_{f} e_{f}^{2} \int_{0}^{1} d z \Theta\left(\kappa_{f}^{2}\right) z(1-z) f_{L}(z) I_{0}\left(\kappa_{f}, \epsilon_{f}\right)$,
with
$\varepsilon_{f}^{2}(z)=z(1-z) Q^{2}+m_{f}^{2}, \kappa_{f}^{2}(z)=z(1-z) M_{X}^{2}-m_{f}^{2}, \quad f_{T}(z)=z^{2}+(1-z)^{2}, \quad f_{L}(z)=4 z^{2}(1-z)^{2}$.
The $x_{\mathbb{P}}$ dependence comes in the functions $I_{\lambda}$ from $N_{A}\left(r, b, x_{\mathbb{P}}\right)$, the $q \bar{q}$ dipole-nucleus scattering amplitude:

$$
\begin{equation*}
I_{\lambda}(\kappa, \epsilon)=\int d^{2} b\left[\int_{0}^{\infty} r d r J_{\lambda}(\kappa r) K_{\lambda}(\epsilon r) N_{A}\left(r, b, x_{\mathbb{P}}\right)\right]^{2} \tag{5.64}
\end{equation*}
$$

where $J_{\lambda}$ and $K_{\lambda}$ are Bessel functions. In equation (5.64), the integration variables $r$ and $b$ are the $q \bar{q}$-dipole transverse size and its impact parameter.

In principle, it is justified to neglect final states containing gluons, because these are suppressed by extra powers of $\alpha_{s}$. However, for small values of $\beta$ or large values of $Q^{2}$, the $q \bar{q}$ pair will emit soft or collinear gluons whose emissions are accomponied by large logarithms $\ln (1 / \beta)$ or $\ln \left(Q^{2}\right)$ which compensate the factors of $\alpha_{s}$. In those situations, multiple gluon emissions should be re-summed; in practice, including the $q \bar{q} g$ final state is enough to describe the HERA data. In both the small- $\beta$ and large $-Q^{2}$ limits, this can be done within the dipole picture. An implementation of the $q \bar{q} g$ contribution $F_{T}^{q \bar{q} g}$ that correctly reproduces both limits was recently proposed [876], while at large $\beta$ and small $Q^{2}$, the $q \bar{q}$ contributions in equation (5.62) dominate. The formulae that we shall use can be found in ref. [876].

The dipole-nucleus scattering amplitude: We shall use the IPsat parametrization to describe the dipole-nucleus scattering amplitude:

$$
\begin{equation*}
N_{A}(r, b, x)=1-e^{-r^{2} F(r, x) \sum_{i=1}^{A} T_{p}\left(b-b_{i}\right)}, \quad F\left(x, r^{2}\right)=\frac{\pi^{2}}{2 N_{c}} \alpha_{s}\left(\mu_{0}^{2}+\frac{C}{r^{2}}\right) x g\left(x, \mu_{0}^{2}+\frac{C}{r^{2}}\right) . \tag{5.65}
\end{equation*}
$$

This is a model of a nucleus whose nucleons interact independently. Indeed, $N_{A}$ is obtained from $A$ dipole-nucleon amplitudes $N_{p}=1-\exp \left[-r^{2} F(r, x) T_{p}(b)\right]$ assuming that the probability $1-N_{A}$ for the dipole not to interact with the nucleus is the product of the probabilities $1-N_{p}$ for the dipole not to interact with the nucleons. This assumption is not consistent with the CGC quantum evolution, which sums up nonlinear interactions between the nucleons. However, the classical limit of the dipole-CGC scattering amplitude can be thought of an initial condition (5.65). Note that in the small $r$ limit, one has $N_{A}=\sum_{i} N_{p}$, and there is no leading twist shadowing.

In (5.65), $T_{p}(b) \propto \exp \left[-b^{2} /\left(2 B_{G}\right)\right]$ is the impact parameter profile function in the proton with $\int d^{2} b T_{p}(b)=1$, and $F$ is proportional to the DGLAP evolved gluon distribution. The parameters $\mu_{0}, C$, and $B_{\mathrm{G}}$ (as well as two other parameters characterising the initial condition for the DGLAP evolution) are fit to reproduce the HERA data on the inclusive proton


Figure 5.32. Left plot: $\beta$-dependence of the different contributions to the proton diffractive structure function $F_{2, p}^{D}$. Right plot: the ratio $F_{2, A}^{D} /\left(A F_{2, p}^{D}\right)$ as a function of $\beta$ for Ca , Sn and Au nuclei. In both cases, results are for the "non breakup" case, and at $Q^{2}=5 \mathrm{GeV}^{2}$ and $x_{\mathbb{P}}=0.001$.
structure function $F_{2}$. The diffractive proton structure function $F_{2}^{D}$ is well reproduced 825] after adjusting $\alpha_{s}=0.14$ in the $q \bar{q} g$ component. Vector-meson production at HERA is also well described. 823

We introduced in (5.65) the coordinates of the individual nucleons $\left\{b_{i}\right\}$, they are distributed according to the Woods-Saxon distribution $T_{A}\left(b_{i}\right)$, which means that to compute an observable, one has to perform the following average

$$
\begin{equation*}
\langle\mathcal{O}\rangle_{N} \equiv \int\left(\prod_{i=1}^{A} d^{2} b_{i} T_{A}\left(b_{i}\right)\right) \mathcal{O}\left(\left\{b_{i}\right\}\right) . \tag{5.66}
\end{equation*}
$$

The Woods-Saxon parameters are measured from the electrical charge distribution, no additional parameters are introduced. The resulting dipole cross sections give a good agreement [826] with the small-x NMC data on the nuclear structure function $F_{2, A}$. We will use this parametrization of $N_{A}$ to predict the nuclear diffractive structure function $F_{2, A}^{D}$.

Note that performing the average at the level of the amplitude (5.66), meaning calculating $\left\langle N_{A}\right\rangle_{N}^{2}$ in (5.62), imposes that the nucleus is intact in the final state. By contrast, when performing the average at the level of the cross-section, meaning calculating $\left\langle N_{A}^{2}\right\rangle_{N}$ in (5.62), one allows the nucleus to break up into individual nucleons, which will typically happen when the momentum transfer is bigger than the inverse nuclear radius. In what follows, we shall refer to those possibilities as "non breakup" and "breakup" cases.

Nuclear enhancement and suppression of $F_{2}^{D}$ : In fig. 5.32, the $\beta$ dependence of the diffractive structure function is displayed for $Q^{2}=5 \mathrm{GeV}^{2}$ and $x_{\mathbb{P}}=0.001$. In the left plot, the hierarchy of the different contributions is analysed in the case of $F_{2, p}^{D}$. The dominant contribution is: the $q \bar{q} g$ component for values of $\beta<0.1$, the longitudinally polarized $q \bar{q}$ component for values of $\beta>0.9$, and the transversely polarized $q \bar{q}$ component for intermediate values. In the case of $F_{2, A}^{D}$, this separation is still true but the $q \bar{q}$ and $q \bar{q} g$ components behave differently as a function of $A$. The $q \bar{q}$ components are enhanced compared to $A$ times the proton diffractive structure functions while the $q \bar{q} g$ component, on the contrary, is suppressed for nuclei compared to the proton (the $Q^{2}$ and $x_{\mathbb{P}}$ dependence of these effects will be discussed shortly).

This leads to a nuclear suppression of the diffractive structure function in the small $\beta$ region, and to an enhancement at large $\beta$. This is illustrated by the right plot of fig. 5.32, where the ratio $F_{2, A}^{D} /\left(A F_{2, p}^{D}\right.$ ) is shown as a function of $\beta$ for different nuclei (for the "non


Figure 5.33. The ratios $F_{2, A}^{D, x} /\left(A F_{2, p}^{D, x}\right)$ of the different components $(x=q \bar{q} g, q \bar{q} T, q \bar{q} L)$ of the diffractive structure function for both "breakup" and "non breakup" cases. Left plot: as a function of $Q^{2}$ for $x_{\mathbb{P}}=0.001$. Right plot: as a function of $x_{\mathbb{P}}$ for $Q^{2}=5 \mathrm{GeV}^{2}$. In both cases, results are for Au nuclei and the different components are evaluated where they are dominant: at $\beta=0.1$ for $q \bar{q} g$, $\beta=0.5$ for $q \bar{q} T$ and $\beta=0.9$ for $q \bar{q} L$.
breakup" case). The net result of the different contributions is that $F_{2, A}^{D} / A$, for a large $\beta$ range down to 0.1 , is close to $F_{2, p}^{D}$, and is increasing with $A$.

In fig. 5.33, for the Au nucleus case, the ratios $F_{2, A}^{D} /\left(A F_{2, p}^{D}\right)$ of individual contributions are analyzed (for values of $\beta$ at which they are dominant). Comparisons between the "breakup" and "non breakup" cases are made, as functions of $Q^{2}$ (left plot) and $x_{\mathbb{P}}$ (right plot). For the $q \bar{q} g$ component, the nuclear suppression is almost constant (the suppression goes away slowly with $Q^{2}$ ). For the $q \bar{q}$ components, the enhancement becomes bigger with increasing $Q^{2}$ and $x_{\mathbb{P}}$. The result for the total diffractive cross-section in e +A scattering is that it decreases more slowly with increasing $Q^{2}$ or $x_{\mathbb{P}}$ compared to the e+p case. Finally, cross sections in the "non breakup" case are about $15 \%$ lower than in the "breakup" case.

Comparing with other approaches, we obtain similar features. We notice one interesting difference with the results obtained using diffractive parton distributions modified by leading twist shadowing [812]: even at large $\beta$, it is found that $F_{2, A}^{D} / A$ is suppressed compared to $F_{2, p}^{D}$ as a function of $Q^{2}$. This could be tested with measurements at a future EIC where diffraction will be an important part of a rich program. A typical nuclear enhancement of diffraction, for a Au nucleus, is a factor of $\sim 1.2$. Combining this with the typical nuclear suppression in the inclusive case $(\sim 0.8$, see 826$)$, we expect the fraction of diffractive events to be increased by a factor of $\sim 1.5$ compared to the proton, meaning 25 to $35 \%$ at the EIC.

## Expectations for diffraction e+A DIS from LT shadowing

## Vadim Guzey and Mark Strikman

The leading twist theory of nuclear shadowing (see section 5.2) that uses the connection between nuclear shadowing and diffraction [791] and allows one to predict nuclear parton distributions (PDFs) at small $x$ [803, 805, 806, 807] can also be used to predict nuclear diffractive PDFs and diffractive structure functions 812 . At small $x$ and in the nuclear target rest frame, the virtual photon interacts coherently with all nucleons of the nuclear target and the $\gamma^{*} A \rightarrow X A$ scattering amplitude is given by the sum of the multiple scattering contributions presented in Fig. 5.34. Graphs $a, b$, and $c$ correspond to the coherent
interaction with one, two, and three nucleons of the nuclear target, respectively: graph $a$ is the impulse approximation; graphs $b$ and $c$ contribute to the shadowing correction. Note that the interactions with four and more nucleons (at the amplitude level) are not shown, but they are implied. The application of the Abramovsky-Gribov-Kancheli (AGK) cutting rules [804] allows one to relate these diagrams to the corresponding diagrams for the total cross section in $\gamma^{*} A$ scattering.


Figure 5.34. The multiple scattering series for the $\gamma^{*} A \rightarrow X A$ diffractive scattering amplitude. Graph $a$ is the impulse approximation; graphs $b$ and $c$ correspond to the interaction with two and three nucleons of the nuclear target, and contribute to the shadowing correction.

Combining the Glauber-Gribov multiple scattering formalism for the $\gamma^{*} A \rightarrow X A$ scattering amplitude with the QCD factorization theorem [808], one can derive the nuclear diffractive parton distribution of flavor $j$ [807, 812]:

$$
\begin{align*}
\beta f_{j / A}^{D(3)}\left(\beta, Q_{0}^{2}, x_{\mathbb{P}}\right) & =4 \pi A^{2} \beta f_{j / N}^{D(4)}\left(\beta, Q_{0}^{2}, x_{\mathbb{P}}, t_{\min }\right) \int d^{2} b \\
& \times\left|\int_{-\infty}^{\infty} d z e^{i x_{\mathbb{P}} m_{N} z} e^{-\frac{A}{2}(1-i \eta) \sigma_{\text {soft }}^{j}\left(x, Q_{0}^{2}\right) \int_{z}^{\infty} d z^{\prime} \rho_{A}\left(b, z^{\prime}\right)} \rho_{A}(b, z)\right|^{2} \tag{5.67}
\end{align*}
$$

where the notation is the same as in eqs. (5.32) and (5.33).
While at the level of the interaction with two nucleons (graphs $a$ and $b$ in fig. 5.34) our predictions are model-independent, the contribution of the interaction with $N \geq 3$ nucleons requires additional model-dependent considerations since these interactions probe the details of the diffractive dynamics beyond what is encoded in the elementary diffractive distribution $f_{j}^{D(4)}$, as discussed in Section 5.2. Viewing the hard probe (virtual photon) as a coherent superposition of the configurations that interact with the target nucleons with very different strengths (from align-jet configurations to point-like configurations) and which are present in the virtual photon with the probability $P(\sigma)$, one immediately sees from fig. 5.34 that diffractive scattering probes all moments of the cross section (color) fluctuations of the virtual photon, $\left\langle\sigma^{n}\right\rangle \equiv \int d \sigma P(\sigma) \sigma^{n}$, up to the order $n=2 A$. One should note that coherent diffraction probes these fluctuations differently from inclusive scattering. For instance, while the shadowing correction to the deuteron's usual parton distributions is proportional to $\left\langle\sigma^{2}\right\rangle$ (i.e., it is unambiguously expressed in terms of the corresponding diffractive PDFs, see eq. 5.32 in section (5.2), the shadowing correction to the deuteron's diffractive PDFs is proportional to $\left\langle\sigma^{3}\right\rangle$ (interference of graphs $a$ and $b$ in fig. 5.34). (Note that the square of graph $b$ in fig. 5.34 proportional to $\left\langle\sigma^{4}\right\rangle$ also contributes, but its contribution is numerically very small.) As the cross section fluctuations of the virtual photon ( $\left\langle\sigma^{n}\right\rangle$ moments) are rather weakly constrained by the present data, predictions of the leading twist theory of nuclear shadowing contain unavoidable theoretical uncertainty associated with modeling of $\left\langle\sigma^{n}\right\rangle$ with $n \geq 3$. Precise measurements of the $t$ dependence of nuclear shadowing in $e D$ diffraction at an EIC will dramatically reduce this uncertainty by determining exactly these moments.

Equation (5.67) determines nuclear diffractive PDFs at a certain initial scale $Q_{0}^{2}$ $\left(Q_{0}^{2}=4 \mathrm{GeV}^{2}\right.$ in our case). As a consequence of QCD factorization [808, the subsequent $Q^{2}$ evolution is given by the DGLAP evolution equations (at fixed $x_{\mathbb{P}}$ and $t$ ). As another consequence of the QCD factorization, the same nuclear diffractive PDFs $f_{j}^{D(3)}$ enter the perturbative QCD description of many processes and observables: the diffractive structure function $F_{2 A}^{D(3)}$, the longitudinal diffractive structure function $F_{L A}^{D(3)}$, the charm structure functions $F_{2 A}^{D(3)(c)}$ and $F_{L A}^{D(3)(c)}$, and diffractive electroproduction of jets and heavy flavors.


Figure 5.35. The leading twist theory of nuclear shadowing predictions for the ratio of nuclear to nucleon gluon and $\bar{u}$ quark diffractive PDFs, $f_{j / A}^{D(3)} /\left(A f_{j / N}^{D(3)}\right)$, as a function of $\beta$ at $x_{\mathbb{P}}=10^{-3}$ and $Q_{0}^{2}=4 \mathrm{GeV}^{2}$. The two sets of curves (labeled FGS10_H and FGS10_L) correspond to the two extreme scenarios of nuclear shadowing.

As an example of our predictions for nuclear diffractive PDFs, in fig. 5.35 we present the ratio of the nuclear ( ${ }^{40} \mathrm{Ca}$ and ${ }^{208} \mathrm{~Pb}$ ) to nucleon diffractive PDFs, $f_{j / A}^{D(3)} /\left(A f_{j / N}^{D(3)}\right)$, as a function of $\beta$ at fixed $x_{\mathbb{P}}=10^{-3}$ and $Q_{0}^{2}=4 \mathrm{GeV}^{2}$. The left column of panels corresponds to the $\bar{u}$-quark distribution; the right column corresponds to the gluon distribution. The two sets of curves (labeled FGS10_H and FGS10_L) correspond to the two scenarios for the effective cross section $\sigma_{\text {soft }}^{j}$, which also determines shadowing effects as discussed in Section 5.2. As one can see from the comparison of fig. 5.35 to our predictions for the usual nuclear PDFs presented in fig. [5.19, nuclear diffractive PDFs are much more sensitive to the effect of the color fluctuations (the spread between the solid and dotted curves is much larger for $f_{j / A}^{D(3)} /\left(A f_{j / N}^{D(3)}\right)$ than for $\left.f_{j / A}\left(x, Q_{0}^{2}\right) /\left[A f_{j / N}\left(x, Q_{0}^{2}\right)\right]\right)$.

| $A /$ model | $F_{2 A, \text { incoh }}^{D(3)} / F_{2 A}^{D(3)}, x_{\mathbb{P}}=10^{-3}$ | $F_{2 A, \text { incoh }}^{D(3)} / F_{2 A}^{D(3)}, x_{\mathbb{P}}=10^{-2}$ |
| :---: | :---: | :---: |
| ${ }^{40} \mathrm{Ca}$, FGS10_H | 0.35 | 0.33 |
| ${ }^{40} \mathrm{Ca}$, FGS10_L | 0.43 | 0.38 |
| ${ }^{208} \mathrm{~Pb}$, FGS10_H | 0.12 | 0.11 |
| ${ }^{208} \mathrm{~Pb}$, FGS10_L | 0.20 | 0.16 |

Table 5.3. The leading twist theory of nuclear shadowing predictions for the ratio of the nuclear structure functions measured in incoherent and coherent diffraction in $e A$ DIS, $F_{2 A \text {,incoh }}^{D(3)} / F_{2 A}^{D(3)}$, at $x_{\mathbb{P}}=10^{-3}$ and $10^{-2}$ and $Q_{0}^{2}=4 \mathrm{GeV}^{2}$. The ratio is approximately $\beta$-independent.

The simplest observable to measure at an EIC is the diffractive structure function $F_{2 A}^{D(3)}$. Our predictions for $F_{2 A}^{D(3)} /\left(A F_{2 N}^{D(3)}\right)$ for $Q^{2} \sim$ few $\mathrm{GeV}^{2}$ are similar in shape and close in
the absolute value for ${ }^{40} \mathrm{Ca}$ and model FGS10_H to the corresponding predictions made in the framework of the color dipole model, where the main contribution originates from the aligned-jet configurations 825. (Note that at the level of the interaction with two nucleons, the expressions for the shadowing correction in our leading twist approach and in the dipole formalism are essentially the same and are unambiguously expressed in terms of $\gamma^{*}$-nucleon diffraction.) Hence, it appears that the $x_{\mathbb{P}}$ and $\beta$ dependence of coherent inclusive diffraction in $e A$ DIS at $Q^{2} \sim Q_{0}^{2}$ may not give unambiguous information on the onset of the non-linear regime of parton dynamics; to distinguish between the nonsaturation and saturation regimes one will need to study the $Q^{2}$ dependence of various diffractive observables.

In addition to inclusive coherent diffraction that we have discussed above, the leading twist theory of nuclear shadowing makes predictions for incoherent diffraction (with nuclear break-up into its constituents) in $e A$ DIS, see [807] for details. An example of our predictions for the ratio of the nuclear structure functions measured in incoherent and coherent diffraction in $e A$ DIS at $x_{\mathbb{P}}=10^{-3}$ and $x_{\mathbb{P}}=10^{-2}$ and $Q_{0}^{2}=4 \mathrm{GeV}^{2}$ is presented in table 5.3. To a good accuracy, the ratio is approximately $\beta$-independent.

## $5.5 k_{T}$-dependent gluons: SIDIS and jets

## Dijet and Dihadron production at EIC

Fabio Dominguez, Cyrille Marquet, Bowen Xiao and Feng Yuan
Dijet production at an EIC: The operator definition of the Weizsäcker-Williams (WW) gluon distribution can be written as follows [267, 283]:

$$
\begin{equation*}
x G^{(1)}\left(x, k_{\perp}\right)=2 \int \frac{d \xi^{-} d \xi_{\perp}}{(2 \pi)^{3} P^{+}} e^{i x P^{+} \xi^{-}-i k_{\perp} \cdot \xi_{\perp}}\langle P| \operatorname{Tr}\left[F^{+i}\left(\xi^{-}, \xi_{\perp}\right) \mathcal{U}^{[+\rfloor \dagger} F^{+i}(0) \mathcal{U}^{[+]}\right]|P\rangle, \tag{5.68}
\end{equation*}
$$

where the gauge $\operatorname{link} \mathcal{U}_{\xi}^{[+]}=U^{n}[0,+\infty ; 0] U^{n}\left[+\infty, \xi^{-} ; \xi_{\perp}\right]$ represents final state interactions with $U^{n}$ being the light-like Wilson line in covariant gauge. By choosing the light-cone gauge with certain boundary conditions for the gauge potential $\left(A_{\perp}\left(\zeta^{-}=\infty\right)=0\right.$ for the specific case above), we can drop out the gauge link contribution in equation (5.68) and find that this gluon distribution has the number density interpretation. Then, it can be calculated from the wave functions or the WW field of the nucleus target [729, 731, 877]. At small- $x$ for a large nucleus, it was found

$$
\begin{equation*}
x G^{(1)}\left(x, k_{\perp}\right)=\frac{S_{\perp}}{\pi^{2} \alpha_{s}} \frac{N_{c}^{2}-1}{N_{c}} \int \frac{d^{2} r_{\perp}}{(2 \pi)^{2}} \frac{e^{-i k_{\perp} \cdot r_{\perp}}}{r_{\perp}^{2}}\left(1-e^{-\frac{r_{\perp}^{2} Q_{s}^{2}}{4}}\right), \tag{5.69}
\end{equation*}
$$

where $N_{c}=3$ is the number of colors, $S_{\perp}$ is the transverse area of the target nucleus, and $Q_{s}^{2}=\frac{g^{2} N_{c}}{4 \pi} \ln \frac{1}{r_{\perp}^{2} \lambda^{2}} \int d x^{-} \mu^{2}\left(x^{-}\right)$is the gluon saturation scale with $\mu^{2}$ the color charge density in a large nuclei.

The second gluon distribution, the Fourier transform of the dipole cross section, is defined in the fundamental representation

$$
\begin{equation*}
x G^{(2)}\left(x, k_{\perp}\right)=2 \int \frac{d \xi^{-} d \xi_{\perp}}{(2 \pi)^{3} P^{+}} e^{i x P^{+} \xi^{-}-i k_{\perp} \xi_{\perp}}\langle P| \operatorname{Tr}\left[F^{+i}\left(\xi^{-}, \xi_{\perp}\right) \mathcal{U}^{[-] \dagger} F^{+i}(0) \mathcal{U}^{[+]}\right]|P\rangle \tag{5.70}
\end{equation*}
$$

where the gauge link $\mathcal{U}_{\xi}^{[-]}=U^{n}[0,-\infty ; 0] U^{n}\left[-\infty, \xi^{-} ; \xi_{\perp}\right]$ stands for initial state interactions. It has been shown in ref. [283] that the Weizsäcker-Williams gluon distribution can be directly probed in the dijet production processes in DIS while the second gluon distribution enters in the total and semi-inclusive DIS cross sections. The quark-antiquark dijet cross section in DIS can be calculated in both the CGC formalism and the TMD approach. In the CGC formalism, the photon splits into a quark-antiquark pair which subsequently undergoes multiple interactions with the nucleus (see figure 5.36 left).

After averaging over the photon's polarization and summing over the quark and antiquark colors and helicities in the splitting functions $\psi_{\alpha \beta}^{T, L \lambda}\left(p^{+}, z, r\right)$, we obtain,

$$
\begin{align*}
\frac{d \sigma^{\gamma_{T, L}^{*} A \rightarrow q \bar{q} X}}{d^{3} k_{1} d^{3} k_{2}}= & N_{c} \alpha_{e m} e_{q}^{2} \delta\left(p^{+}-k_{1}^{+}-k_{2}^{+}\right) \int \frac{\mathrm{d}^{2} x_{1}}{(2 \pi)^{2}} \frac{\mathrm{~d}^{2} x_{1}^{\prime}}{(2 \pi)^{2}} \frac{\mathrm{~d}^{2} x_{2}}{(2 \pi)^{2}} \frac{\mathrm{~d}^{2} x_{2}^{\prime}}{(2 \pi)^{2}} \\
& \times e^{-i k_{1 \perp} \cdot\left(x_{1}-x_{1}^{\prime}\right)} e^{-i k_{2 \perp} \cdot\left(x_{2}-x_{2}^{\prime}\right)} \sum_{\lambda \alpha \beta} \psi_{\alpha \beta}^{T, L \lambda}\left(x_{1}-x_{2}\right) \psi_{\alpha \beta}^{T, L \lambda *}\left(x_{1}^{\prime}-x_{2}^{\prime}\right) \\
& \times\left[1+S_{x_{g}}^{(4)}\left(x_{1}, x_{2} ; x_{2}^{\prime}, x_{1}^{\prime}\right)-S_{x_{g}}^{(2)}\left(x_{1}, x_{2}\right)-S_{x_{g}}^{(2)}\left(x_{2}^{\prime}, x_{1}^{\prime}\right)\right] \tag{5.71}
\end{align*}
$$

where $k_{1}$ and $k_{2}$ are momenta for the final state quark and antiquark, respectively. We further define $\vec{P}_{\perp}=\vec{k}_{1 \perp}-\vec{k}_{2 \perp}$ and $\vec{q}_{\perp}=\vec{k}_{1 \perp}+\vec{k}_{2 \perp}$. All transverse momenta are defined



Figure 5.36. Left: Typical diagrams contributing to the cross section in the DIS at small- $x$ limit. Right: EIC dihadron correlation function
in the center of mass frame of the virtual photon and the nucleus target. The two- and four-point functions are defined as
$S_{x_{g}}^{(2)}\left(x_{1}, x_{2}\right)=\frac{1}{N_{c}}\left\langle\operatorname{Tr} U\left(x_{1}\right) U^{\dagger}\left(x_{2}\right)\right\rangle_{x_{g}}, S_{x_{g}}^{(4)}\left(x_{1}, x_{2} ; x_{2}^{\prime}, x_{1}^{\prime}\right)=\frac{1}{N_{c}}\left\langle\operatorname{Tr} U\left(x_{1}\right) U^{\dagger}\left(x_{1}^{\prime}\right) U\left(x_{2}^{\prime}\right) U^{\dagger}\left(x_{2}\right)\right\rangle_{x_{g}}$.
The notation $\langle\ldots\rangle_{x_{g}}$ is used for the CGC average of the color charges over the nuclear wave function where $x_{g}$ is the smallest fraction of longitudinal momentum probed, and is determined by the kinematics.

In order to simplify the above result and obtain a factorized expression, we take the correlation limit of equation (5.71). For convenience, we introduce the transverse coordinate variables: $u=x_{1}-x_{2}$ and $v=z x_{1}+(1-z) x_{2}$, and similarly for the primed coordinates. The respective conjugate momenta are $\tilde{P}_{\perp}=(1-z) k_{1 \perp}-z k_{2 \perp} \approx P_{\perp}$ and $q_{\perp}$, and therefore the correlation limit $\left(\tilde{P}_{\perp} \gg q_{\perp}\right)$ can be taken by assuming $u$ and $u^{\prime}$ are small and then expanding the integrand with respect to these two variables before performing the Fourier transform. Therefore, we can obtain the following expression which agrees perfectly with the TMD approach:

$$
\begin{equation*}
\frac{d \sigma_{\mathrm{TMD}}^{\gamma_{T, L}^{*} A \rightarrow q \bar{q}+X}}{d \mathcal{P} . \mathcal{S} .}=\delta\left(x_{\gamma^{*}}-1\right) x_{g} G^{(1)}\left(x_{g}, q_{\perp}\right) H_{\gamma_{T, L}^{*} g \rightarrow q \bar{q}}, \tag{5.73}
\end{equation*}
$$

where $x_{g}$ is the momentum fraction carried by the gluon and is determined by the kinematics, $x_{\gamma^{*}}=z_{q}+z_{\bar{q}}$ with $z_{q}=z$ and $z_{\bar{q}}=1-z$ being the momentum fractions of the virtual photon carried by the quark and antiquark, respectively. The phase space factor is defined as $d \mathcal{P} . \mathcal{S}$. $=d y_{1} d y_{2} d^{2} P_{\perp} d^{2} q_{\perp}$, and $y_{1}$ and $y_{2}$ are rapidities of the two outgoing particles in the lab frame. The leading order hard partonic cross section reads

$$
\begin{equation*}
H_{\gamma_{T}^{*} g \rightarrow q \bar{q}}=\alpha_{s} \alpha_{e m} e_{q}^{2} \frac{\hat{s}^{2}+Q^{4}}{\left(\hat{s}+Q^{2}\right)^{4}}\left(\frac{\hat{u}}{\hat{t}}+\frac{\hat{t}}{\hat{u}}\right), \quad H_{\gamma_{L}^{*} g \rightarrow q \bar{q}}=\alpha_{s} \alpha_{e m} e_{q}^{2} \frac{8 \hat{s} Q^{2}}{\left(\hat{s}+Q^{2}\right)^{4}}, \tag{5.74}
\end{equation*}
$$

with the usually defined partonic Mandelstam variables $\hat{s}=P_{\perp}^{2} /(z(1-z)), \hat{t}=-\left(P_{\perp}^{2}+\right.$ $\left.\epsilon_{f}^{2}\right) /(1-z)$, and $\hat{u}=-\left(P_{\perp}^{2}+\epsilon_{f}^{2}\right) / z$ with $\epsilon_{f}^{2}=z(1-z) Q^{2}$.
di-hadron correlations in DIS: By including the $k_{t}$ dependent fragmentation functions as proposed in ref. [332, one can compute the di-hadron production cross section and the
correlation function $C\left(\phi_{12}\right)$ which is defined as follows

$$
\begin{equation*}
C\left(\phi_{12}\right)=\frac{1}{\frac{d \sigma_{\mathrm{tot} \sin 1 S}^{*}}{d z_{h 1}}} \frac{d \sigma_{\mathrm{tot}}^{\gamma^{*} A \rightarrow h_{1} h_{2}+X}}{d z_{h 1} d z_{h 2} d \phi_{12}}, \tag{5.75}
\end{equation*}
$$

where $z_{h 1}$ and $z_{h 2}$ are the longitudinal momentum fractions of two produced hadrons w.r.t. the photon momentum. $p_{1 \perp}$ and $p_{2 \perp}$ are the transverse momenta of these two back-toback hadrons and $\phi_{12}$ is the azimuthal angle between them. Thus, it is straightforward to numerically evaluate the correlation function and plot it in figure 5.36 right, where we fix $z_{h 1}=z_{h 2}=0.3, Q^{2}=4.0 \mathrm{GeV}^{2}, \sqrt{s}=100 \mathrm{GeV} . p_{1 \perp}$ and $p_{2 \perp}$ are integrated in the range $[2,3] \mathrm{GeV}$ and $[1,2] \mathrm{GeV}$, respectively. For the gluon distribution in gold nuclei, we have used a parametrization inspired by $G B W$ model. From figure 5.36, one sees the suppression of the away-side peak in nuclei due to gluon saturation.

Conclusion: First of all, we would like to compare the dijet production process in DIS to the inclusive and semi-inclusive DIS. As shown above, we derive that the dijet production cross section in DIS is proportional to the WW gluon distribution in the correlation limit. On the other hand, it is well-known that inclusive and semi-inclusive DIS involves the dipole cross section instead [878], which can be related to the second gluon distribution. This might look confusing at first sight, so let us take a closer look at equation (5.71). If one integrates over one of the outgoing momenta, say $k_{1}$, one can easily see that the corresponding coordinates in the amplitude and conjugate amplitude are identified ( $x_{1}=x_{1}^{\prime}$ ) and, therefore, the four-point function $S_{x_{g}}^{(4)}\left(x_{1}, x_{2} ; x_{2}^{\prime}, x_{1}^{\prime}\right)$ collapses to a two-point function $S_{x_{g}}^{(2)}\left(x_{2}, x_{2}^{\prime}\right)$. As a result, the SIDIS and inclusive DIS cross section only depend on two-point functions, thus they only involve the dipole gluon distribution.

Now we can see the unique feature of the dijet production process in DIS. By keeping the momenta of the quark and antiquark unintegrated, we can keep the full color structure of the four-point function which eventually leads to the WW gluon distribution in the correlation limit. Therefore, measuring the dijet production cross sections or dihadron correlations in DIS at future experimental facilities like EIC would give us a first direct and unique opportunity to probe and understand the Weizsäcker-Williams gluon distribution. Last but not least, by measuring the SIDIS and inclusive DIS cross section at EIC, one can also probe and constrain the dipole gluon distribution.

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## Heavy quark production in $e+A$ collisions

## Victor P. Gonçalves

In this contribution we calculate the cross section of heavy quark production using the dipole approach and a nuclear saturation model based on the physics of the Color Glass Condensate (CGC) (For more details and references see Ref. [879]). The main input of our calculation is the dipole-nucleus cross section, $\sigma_{d A}(x, r)$, which is determined by the QCD dynamics at small $x$. In the eikonal approximation it is given by twice the impact-parameter $b$ integral of $\mathcal{N}^{A}(x, r, b)$, the forward dipole-target scattering amplitude for a dipole with size $r$ which encodes all the information about the hadronic scattering, and thus about the
nonlinear and quantum effects in the hadron wave function. In our calculations we will assume as before that the forward dipole-nucleus amplitude is given by

$$
\begin{equation*}
\mathcal{N}^{A}(x, r, b)=1-\exp \left[-\frac{1}{2} \sigma_{d p}\left(x, r^{2}\right) T_{A}(b)\right] \tag{5.76}
\end{equation*}
$$

where $\sigma_{d p}$ is the dipole-proton cross section and $T_{A}(b)$ is the nuclear profile function, which is obtained from a 3-parameter Fermi distribution for the nuclear density normalized to A. It is important to emphasize that this model describes the current experimental data on the nuclear structure function as well as includes the impact parameter dependence in the dipole nucleus cross section. For the dipole-proton cross section we will use the b-CGC model.

To estimate the magnitude of the saturation effects in heavy quark production, let us compare the CGC predictions with those associated to linear QCD dynamics. As a model for the linear regime we consider the leading logarithmic approximation for the dipole-target cross section, where $\sigma_{d A}$ is directly related to the nuclear gluon distribution $x g_{A}$ as follows

$$
\begin{equation*}
\sigma_{d A}\left(x, r^{2}\right)=\frac{\pi^{2}}{3} r^{2} \alpha_{s} x g_{A}\left(x, 10 / r^{2}\right) \tag{5.77}
\end{equation*}
$$

The use of this cross section in the formulae given below will produce results which we denote CT, from color transparency. In this limit we are disregarding multiple scatterings of the dipole with the nuclei and are assuming that the dipole interacts incoherently with the target. In what follows we consider two different models for the nuclear gluon distribution. In the first one we disregard the nuclear effects and assume that $x g_{A}\left(x, Q^{2}\right)=A \cdot x g_{N}\left(x, Q^{2}\right)$, with $x g_{N}$ being the gluon distribution in the proton and given by the GRV98 parameterization. We will refer to this model as CT. In the second model we take into account the nuclear effects in the nuclear gluon distribution as described by the EKS98 parameterization. We will call this model CT + Shad. In our calculations the charm quark mass is $m_{c}=1.5 \mathrm{GeV}$ and the bottom quark mass is $m_{b}=4.5 \mathrm{GeV}$.

Heavy quark production in the color dipole approach: Heavy quark production is usually estimated using the collinear factorization approach, where all partons involved are assumed to be on mass shell, carrying only longitudinal momenta, and their transverse momenta are neglected in the QCD matrix elements. On the other hand, in the large energy (small-x) limit, we have that the characteristic scale $\mu$ of the hard subprocess of parton scattering is much less than $\sqrt{s}$, but greater than the $\Lambda_{Q C D}$ parameter. In this limit, the effects of the finite transverse momenta of the incoming partons become important, and the factorization must be generalized, implying that the cross sections are now $k_{\perp}$-factorized into an off-shell partonic cross section and a $k_{\perp}$-unintegrated parton density function $\mathcal{F}\left(x, k_{\perp}\right)$, characterizing the $k_{\perp}$-factorization approach. Recently, an alternative approach to calculating the heavy quark production at high energies was proposed, considering the quasi-multi-Regge-kinematics (QMRK) framework. It is based on an effective theory implemented with the non-Abelian gauge-invariant action. The heavy quark production can also be calculated using the color dipole approach. This formalism can be obtained from the $k_{\perp}$-factorization approach after the Fourier transformation from the space of quark transverse momenta into the space of transverse coordinates. It is important to emphasize that this equivalence is only valid in the leading logarithmic approximation, being violated if the exact gluon kinematics is considered. A detailed discussion of the equivalence or


Figure 5.37. Transverse momentum charm spectrum (left) and bottom spectrum (right) for $Q^{2}=2$ $\mathrm{GeV}^{2}$ and different energies.
not between the dipole and the QMRK approaches still is an open question. The main advantage to use the color dipole formalism, is that it gives a simple unified picture of inclusive and diffractive processes and the saturation effects can be easily implemented in this approach.

In the color dipole approach, the heavy quark production cross section is given by

$$
\begin{align*}
\frac{d \sigma\left(\gamma^{*} A \rightarrow Q X\right)}{d^{2} p_{Q}^{\perp}} & =\frac{6 e_{Q}^{2} \alpha_{e m}}{(2 \pi)^{2}} \int d \alpha\left\{\left[m_{Q}^{2}+4 Q^{2} \alpha^{2}(1-\alpha)^{2}\right]\left[\frac{I_{0}}{p_{Q}^{\perp 2}+\epsilon^{2}}-\frac{I_{2}}{4 \epsilon}\right]\right. \\
& \left.+\left[\alpha^{2}+(1-\alpha)^{2}\right]\left[\frac{p_{Q}^{\perp} \epsilon I_{1}}{p_{Q}^{\perp 2}+\epsilon^{2}}-\frac{I_{0}}{2}+\frac{\epsilon I_{2}}{4}\right]\right\} \tag{5.78}
\end{align*}
$$

with

$$
I_{\lambda}=\int d r r J_{\lambda}\left(p_{Q}^{\perp} r\right) K_{\lambda}(\epsilon r) \sigma_{d A}(r) ; I_{2}=\int d r r^{2} J_{0}\left(p_{Q}^{\perp} r\right) K_{1}(\epsilon r) \sigma_{d A}(r)
$$

with $\lambda=0,1$, and $J_{0,1}$ and $K_{0,1}$ are Bessel functions, and $\epsilon^{2}=\alpha(1-\alpha) Q^{2}+m^{2}$.


Figure 5.38. Dependence on the photon virtuality at $p_{T}^{2}=4 \mathrm{GeV}^{2}$.
Results: In Fig. 5.37 we show the transverse momentum spectrum of charm quarks. The main purpose of this figure is to show that the predictions of the linear physics (CT +

Shad) differ from the total (i.e. bCGC) by a factor which increases with the energy $W$ and goes from $1.5(W=100 \mathrm{GeV})$ to $4(W=1400 \mathrm{GeV})$. Moreover, this difference persists for a wide momentum window. At very large $p_{T}$ we enter the deep linear regime and expect that the two curves coincide.

In Fig. 5.37 we show the transverse momentum spectrum of bottom quarks. As expected, we observe the same features of the charm distribution, except that now the nonlinear effects are weaker. Nevertheless they are still noticeable. In Fig. 5.38 we show the $Q^{2}$ dependence of the $p_{T}$ distribution at a fixed value $p_{T}=4 \mathrm{GeV}^{2}$ for different energies. The upper and lower panels show the charm and bottom distributions respectively. Here again, we observe a remarkable strength and persistence up to large virtualities of the differences between CT + Shad and bCGC.

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## 5.6 b-dependent gluons: exclusive VM, DVCS

Gluon Density in e+A : KLN, CGC, DGLAP Glauber, or Neither?

William A. Horowitz

Perturbative quantum chromodynamics ( pQCD ) predicts a nontrivial expansion in the size of the nuclear wavefunction at small $x$ as the perturbative power law tails of the gluon distribution near the edge of the nucleus become important compared to the exponential dropoff due to confinement effects [871, 742, 766]. Similarly, in order to not violate unitarity, the enormous growth in the gluon parton distribution function as $x$ becomes small found via naïve application of DGLAP evolution (see [3] and references therein) must be tamed by perturbatively-calculable saturation effects [742, 766]. However it is not yet clear from a theoretical standpoint at what values of $x$ these nontrivial changes in the dominant dynamics occur [766]. Additionally a quantitative theoretical understanding of experimental heavy ion data requires a quantitative understanding of the initial geometry of a heavy ion collision. Certainly observables such as the azimuthal anisotropy of particles [880, 881, 882] are correlated with the anisotropy of the initial geometry; surprisingly the event-by-event fluctuations in the initial geometry also strongly affect these observables [883, 884. In particular the viscosity to entropy ratio $(\eta / s)$ of the quark-gluon plasma (QGP) found by comparing hydrodynamics simulations to heavy ion collision data is directly related to the eccentricity of the initial thermal quark-gluon plasma distribution that is evolved hydrodynamically. Currently the uncertainty in the initial thermal distribution due to the uncertainty in the importance of saturation effects in the initial nuclear profiles is large enough that it is not clear whether the physics of the QGP is better described by leading order weakly-coupled perturbative quantum chromodynamics (LO pQCD) or by LO strongly-coupled anti-deSitter/conformal field theory (AdS/CFT) methods [881. An experimental measurement of the spatial gluon distribution in a highly boosted nucleus, and hence the relevant physics in this kinematic range, would thus be a very interesting and important contribution to our understanding of QCD.

Exclusive vector meson production (EVMP) in e + A collisions has been proposed as a channel for just such a measurement [618, 885, 827]. In this section we will focus on the production of heavy vector mesons, in particular $J / \Psi$ mesons. To leading order, EVMP of a $J / \Psi$ meson occurs in an e + A collision when a photon emitted by the electron splits into a $c-\bar{c}$ pair which communicates with the gluon density in the highly boosted nucleus via a two gluon exchange and subsequently forms a $J / \Psi$ meson and nothing else (we will be interested here in coherent EVMP, in which case the nucleus remains intact); see figure 5.39 for a visualization of the process. It is precisely this two gluon exchange which yields a diffractive measurement of the gluon density in a nucleus.

Previous work [885 explored how modest changes in the Woods-Saxon distribution [886] of a nucleus might manifest themselves as changes in the diffractive peaks in EVMP if one assumes that the spatial distribution of gluons in a nucleus is proportional to the Glauber thickness function found from the Woods-Saxon distribution. That these modest changes do result in a visually obvious modification of the diffraction pattern motivated our further study, in which we consider whether two very different physical pictures of the gluon distribution in a highly boosted nucleus can be experimentally distinguished via EVMP: in particular we wish to compare the diffraction patterns that emerge when the gluon distribution 1) has normalization dictated by DGLAP evolution and spatial distribution
given by the Glauber thickness function and 2) is given by the KLN parameterization (see [887, 888] and references therein) of the Color Glass Condensate (CGC) (see, e.g., [766, 889] for a review). We choose to investigate these two ansätze of the gluon distribution in nuclei as they have been the dominant models used in heavy ion physics calculations to estimate the uncertainty in the viscosity to entropy ratio of the QGP produced at RHIC due to the uncertainty of the currently poorly constrained initial conditions in heavy ion collisions [880, 881].

It is worth taking a moment to comment on some common - yet confusing - terminology in the EVMP field. As mentioned above, to leading order the coherent production of a vector meson in an $\mathrm{e}+\mathrm{A}$ collision involves a two-gluon exchange between the $q-\bar{q}$ pair and the nucleus. If one assumes that all two-gluon exchanges occur independently, then one may exponentiate the single two-gluon exchange result. Making this independence assumption is often referred to in the EVMP field as using "saturation" physics because the cross section is unitarized via the exponentiation process. However this "saturation" does not refer to unitarizing the gluon distribution functions themselves. For instance in the "IP-Sat" 600] and "b-Sat" 823 models, where "Sat" is short for saturation, the $x$ evolution of the gluon PDF is effected through the use of the DGLAP equations. On the other hand, the "b-CGC" model [823] incorporates both the exponentiation of the two-gluon exchange and the CGC physics of the saturation of the gluon PDF. We note that, in principle, small- $x$ evolution effects and exponentiation effects in the dipole cross section should become appreciable simultaneously [737]. In order to (hopefully) make the presentation more clear, and to simplify some of the numerics, we will not exponentiate the two-gluon exchange; we will present results using only the leading order two-gluon exchange in which the gluon PDF is given either via DGLAP evolution or from the CGC. Any subsequent reference to "saturation" in this paper will refer to the saturation of the gluon distribution function alone.

Formalism: Following [600, 885], the diffractive production of a vector meson from a photon scattering off a target is

$$
\begin{equation*}
\frac{d \sigma}{d t}=\frac{1}{16 \pi}\left|\int d^{2} \boldsymbol{r} \int \frac{d z}{4 \pi} \int d^{2} \boldsymbol{b}\langle V \mid \gamma\rangle_{T} e^{i \boldsymbol{b} \cdot \boldsymbol{\Delta}} \frac{d \sigma_{q \bar{q}}}{d^{2} \boldsymbol{b}}\right|^{2} \tag{5.79}
\end{equation*}
$$

where $\langle V \mid \gamma\rangle_{T}$ is the overlap of the vector meson wavefunction and the transversely polarized virtual photon wavefunction - the contribution from the longitudinally polarized photon is zero as we are interested in $Q^{2}=0$ photoproduction-and we used the photon-meson overlap and Gauss-LC model for the $J / \Psi$ wavefunction from [600] ${ }^{5}$, and $\boldsymbol{\Delta}^{2}=-t$. $d \sigma_{q \bar{q}} / d^{2} \boldsymbol{b}$ is the differential cross section for the interaction of the dipole with the target; its form depends on the physics assumptions we make for the nuclear gluon distribution, as we discuss in detail below.

DGLAP Evolution in $x$, Glauber Distribution of Gluons in $b$ : If we assume that the two gluon exchange from the dipole to the nucleus occurs within an individual nucleon then

$$
\begin{equation*}
\frac{d \sigma_{q \bar{q}}}{d^{2} b}=\frac{\pi^{2}}{N_{c}} r^{2} \alpha_{s}\left(\mu^{2}\right) x g\left(x, \mu^{2}\right) T(b), \tag{5.80}
\end{equation*}
$$

[^279]

Figure 5.39. Leading order Feynman diagram for the exclusive vector meson production of a $J / \Psi$ meson.
where $r$ is the size of the dipole, $\mu=\sqrt{ }\left(\mu_{0}+C / r^{2}\right)$ is the relevant momentum scale for the dipole, $x g$ is the gluon distribution function, and

$$
\begin{equation*}
T(b)=\frac{1}{2 \pi B_{G}} e^{-b^{2} / 2 B_{G}} \tag{5.81}
\end{equation*}
$$

is the assumed spatial distribution of gluons in a nucleon. We use the MSTW parameterization of the gluon $\operatorname{PDF}$ [22]. As described in [821], $\mu_{0}$ and $C$ are free parameters; as in [821, 600, 827], we take $\mu_{0}=1 \mathrm{GeV}^{2}$ and $C=4$. From HERA data [588] the measured slope of $d \sigma / d t$ yields $B_{G} \approx 4.25 \mathrm{GeV}^{-2} 600$. Then

$$
\begin{equation*}
\frac{d \sigma^{D G L A P}}{d t}=4 \pi \sigma_{p}^{2} e^{-B_{G} t}\left|\int d b J_{0}(b \sqrt{t}) T_{A}(b)\right|^{2} \tag{5.82}
\end{equation*}
$$

where $J_{0}$ is the usual Bessel function, $T_{A}(b) \equiv \int d z \rho_{A}\left(\sqrt{b^{2}+z^{2}}\right)$, with $\int d^{2} \boldsymbol{b} T_{A}(b)=A$, is the usual thickness function, and $\rho_{A}$ is the density of the nucleus (here taken as the Woods-Saxon distribution of ${ }^{197} \mathrm{Au}$ with the usual $R=6.38 \mathrm{fm}$ and $a=0.535 \mathrm{fm}$ [890]) and

$$
\begin{equation*}
\sigma_{p} \equiv \frac{1}{4 \pi} \int d^{2} \boldsymbol{r} \int d z\langle V \mid \gamma\rangle_{T} \frac{\pi^{2}}{N_{c}} r^{2} \alpha_{s}\left(\mu^{2}\right) x g\left(x, \mu^{2}\right) \tag{5.83}
\end{equation*}
$$

CGC Distribution of Gluons in $x$ and $b$ : Alternatively we may view the nucleus as a whole and that the gluon distribution is found from the CGC. In this case

$$
\begin{equation*}
\frac{d \sigma_{q \bar{q}}}{d^{2} \boldsymbol{b}}=\frac{\pi^{2}}{N_{C}} r^{2} \alpha_{s}\left(\mu^{2}\right) x g_{A}\left(\mu^{2}, Q_{s}^{2}\right) \tag{5.84}
\end{equation*}
$$

where $x g_{A}$ is the integrated gluon distribution function related to the unintegrated gluon distribution (UGD) $\phi_{A}$ by

$$
\begin{equation*}
x g_{A}\left(\mu^{2}, Q_{s}^{2}\right)=\int d^{2} \boldsymbol{k} \phi_{A}\left(k^{2}, Q_{s}^{2}\right)=\pi \int_{0}^{k_{\max }^{2}=\mu^{2}} d k^{2} \phi_{A}\left(k^{2}, Q_{s}^{2}\right) \tag{5.85}
\end{equation*}
$$

The $x$ and $b$ dependence of the two-gluon exchange dipole scattering formula, Eq. 5.84, comes in implicitly through the $x$ and $b$ dependence of $Q_{s}^{2}$ [888,

$$
\begin{equation*}
Q_{s}^{2} \equiv \frac{2 \pi^{2}}{C_{F}} \alpha_{s}\left(Q_{s}^{2}\right) x g\left(x, Q_{s}^{2}\right) T_{A}(b) \tag{5.86}
\end{equation*}
$$

where $C_{F} \equiv\left(N_{c}^{2}-1\right) / 2 N_{c}$.
In principle one determines the UGD via the JIMWLK evolution equations or, in the large- $N_{c}$ limit, the BK evolution equations (see [766, 889$]$ and references therein). However, instead of solving the full evolution equations many heavy ion physics calculations use instead the KLN prescription of the CGC (see, e.g., [887, 888), which attempts to capture the main feature of CGC physics; in particular, the KLN UGD becomes saturated at momenta on the scale of the saturation scale $Q_{s}$. Because of its widespread use in heavy ion physics calculations and in order to simplify our own calculations we, too, will use the KLN UGD,

$$
\phi_{A}^{K L N}\left(k, Q_{s}^{2}\right)=\frac{\kappa C_{F} Q_{s}^{2}}{2 \pi^{3} \alpha_{s}\left(Q_{s}^{2}\right)} \begin{cases}\left(Q_{s}^{2}+\Lambda^{2}\right)^{-1}, & k^{2} \leq Q_{s}^{2}  \tag{5.87}\\ \left(k^{2}+\Lambda^{2}\right)^{-1}, & k^{2}>Q_{s}^{2},\end{cases}
$$

where $\kappa$ is an $O(1)$ parameter meant to represent higher order corrections to the UGD, and $\Lambda=0.2 \mathrm{GeV}$ [888.

In principle $\kappa$ is set by comparing to known experimental observables such as the measured multiplicity at midrapidity at RHIC [891, 892, 893] or LHC [894, 895] or to the diffractive cross sections for protons measured at HERA [588]. However we found that the results from the leading order multiplicity formula [887] are linearly dependent on the cutoff taken for $\alpha_{s}, \alpha_{s}^{\max }$. The KLN UGD itself, though, is not nearly as sensitive to $\alpha_{s}^{\max }$, so the multiplicity prescription does not provide a robust way of setting $\kappa$. We note in passing that the centrality dependence of the particles produced via the leading order CGC multiplicity formula using the KLN UGD's also depends on $\alpha_{s}^{\max }$. Perhaps the use of the next-to-leading order results in the UGD [896] and/or the production formula [897] will mitigate this dependence enough to make reasonable comparisons of CGC multiplicity to current data. Currently, though, there does not appear to be any quantitative estimate of the size of the dependence of the predicted CGC multiplicity as a function of centrality on $\alpha_{s}^{\max }$. $\kappa$ also cannot be set by comparing to the proton diffractive cross section as the currently available data does not probe regions of $x$ small enough such that $Q_{s}^{2}$ is a perturbative scale (at least when using the LO MSTW PDFs). In our calculations we will set $\kappa=1$.

It is important to contrast the interaction of the dipole in the KLN CGC approach taken here, in which the $q-\bar{q}$ pair interacts with the entire nucleus, and the Glauber approach, in which the pair interacts with individual nucleons. By interacting with individual nucleons the diffractive cross section for the DGLAP Glauber model picks up an extra exponential suppression in $t$ proportional to the square of the width of the nucleon, $B_{G}$.

Results: The saturation physics of the CGC has resulted in a wider and flatter gluon distribution than that from the Glauber treatment; the DGLAP growth of the small- $x$ gluon distribution - tamed by the saturation physics of the KLN CGC-leads to a significant enhancement in the cross section at $x=10^{-5}$ compared to that found using the KLN CGC gluon distribution. It is worth noting that the KLN prescription for the CGC satisfies the black disk limit.

We attempt to quantify the changes in both the nuclear gluonic width and density as a function of $x$ and note that even out to extremely small values of $x \sim 10^{-13}, b_{1 / 2}$ from the KLN CGC continues to rise sublinearly with $\log (s)$; thus the implementation of the KLN CGC used here, with the MSTW gluon PDF, satisfies the Froissart bound 871. Intriguingly this sublinear (as opposed to linear) growth in radius as a function of $\log s$ is a surprise compared to other CGC parameterizations [872]. Note the enormous growth of
the dipole cross section as $x$ decreases for the LO DGLAP-evolved gluonic density. This unitarity-violating enhancement is clearly reduced tremendously with the saturation physics of the KLN CGC.

The drastically faster increase in the gluon density from the DGLAP evolved PDF results in a cross section that increases much faster as a function of $x$ than for the KLN CGC case. As was shown in $[827]^{6}$ the incoherent cross section, in which the nucleus breaks up, begins to dominate the total diffractive cross section by $t \sim 0.02 \mathrm{GeV}^{-2}$. It is likely that the $t$ dependence of the incoherent EVMP of the two models will be different, although we do not provide a quantitative estimate here: the decrease in cross section as a function of $t$ for the DGLAP Glauber model will be enhanced by $\exp \left(-B_{G} t\right)$ due to the assumption that the heavy quark dipole interacts with individual nucleons. And in the case of coherent scattering one can discern a stronger $t$ dependence in the DGLAP Glauber results due precisely to the extra $\exp \left(-B_{G} t\right)$ factor that results from treating the nucleus as a collection of individual nucleons. More importantly, the much larger gluon density yields a particularly noticeable difference at $t=0$, where possible nuclear breakup effects are negligible.Even with the very large PDF uncertainties as $x$ decreases, there is a clear increase in the coherent diffractive cross section for the DGLAP Glauber dipole compared to the KLN CGC dipole.
Conclusions and Discussion: An enormous wealth of information on the gluonic structure of highly relativistic nuclei can be found using exclusive vector meson production. In particular we investigated the experimental signatures of the coherent scattering of a $c \bar{c}$ dipole onto a nucleus that results in an intact nucleus and a $J / \Psi$ meson in e + A collisions at eRHIC energies. We found that the diffractive cross section will readily experimentally differentiate between the two common initial highly boosted nucleus prescriptions used in heavy ion physics phenomenology: 1) the gluon density is found using DGLAP evolution and its spatial distribution is assumed to be proportional to the at-rest Glauber nuclear thickness function and 2) the gluon density and distribution is given by the KLN parameterization of the CGC. In particular there is the exciting possibility of literally watching a nucleus grow with center of mass energy as the positions in $t$ of the minima and maxima in the diffractive cross section for the saturation physics calculation depend quite strongly on $\log (x)$. On the other hand the DGLAP Glauber model yields a nucleus of constant size as a function of $x$; the positions in $t$ of the diffractive minima and maxima do not change as a function of $x$. At the same time one is determining the width of a nucleus in $\mathrm{e}+\mathrm{A}$ collisions, one will also measure the $x$ dependence of the normalization of $d \sigma / d t$. Due to the explosion of small- $x$ gluons the DGLAP Glauber approach yields a normalization that rapidly increases as a function of $x$; additionally the $t$ dependence of the DGLAP Glauber $d \sigma / d t$ is also quite strong as it is proportional to $\exp \left(-B_{G} t\right)$ due to the assumption that the $q-\bar{q}$ dipole interacts with individual nucleons. Conversely the KLN CGC dipole description does not have a strong $x$ dependence in its normalization due to its inclusion of saturation effects; similarly, the interaction of the dipole with the whole nuclear gluonic wavefunction yields a weaker $t$ dependence than is displayed by the DGLAP Glauber results.

It is clear that, at the very least, the striking difference between the $x$ dependence of the peaks and minima from the DGLAP Glauber model and the KLN CGC model are robust: these differences will persist should we use even more sophisticated models of these two physical pictures; the $x$ dependence of the peaks and minima will persist should we attempt to approximate multiple scattering within the nucleus by exponentiating the dipole cross

[^280]section, should we use a less approximate CGC calculation such as is found in 896], or should we examine the results from other vector mesons such as the $\phi$ or $\rho$. We regrettably leave the quantification of the diffractive cross section for these more sophisticated physical models and additional vector mesons for future work. Exponentiating the two-gluon exchange cross section will reduce the enormous growth in the diffractive cross section in the DGLAP Glauber picture compared to the CGC case; we suspect this reduction will not be too large, although we also leave the quantification of this reduction to future work.

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## Coherent vs incoherent diffraction

## Tuomas Lappi and Cyrille Marquet

The purpose of this section is to investigate incoherent diffraction in a simpler context than with inclusive diffraction $\gamma^{*} A \rightarrow X Y$, mainly using diffractive vector meson production $\gamma^{*} A \rightarrow V Y$, where the diffractive final state X consists of a vector meson and nothing else, $A$ stands for the target nucleus and $Y$ for the final state it may dissociate into. At high energies, the $q \bar{q}$ dipole that the virtual photon has fluctuated into, scatters off the gluonic field of the nucleus before recombining into the vector meson. While this scattering involves a color-singlet exchange, leaving a rapidity gap in the final state, the nucleus can still interact elastically ( $Y=A$, this is called coherent diffraction) or inelastically (i.e. break up, called incoherent diffraction). In this process, the momentum transfer $t$ can be determined from the meson regardless of the fate of the target, and elastic and inelastic interactions of the target can be experimentally distinguished.

Kinematically, a low invariant mass of the system $Y$ corresponds to a large rapidity gap in the final state between that system and the vector meson, and implies that the longitudinal momentum of the meson is close to that of the incoming photon. In this case, the eikonal approximation can be assumed to compute the dipole-nucleus scattering. At small values of $x=\left(Q^{2}+M_{V}^{2}\right) /\left(Q^{2}+W^{2}\right)$ where $Q^{2}$ is the photon virtuality, $M_{V}$ the vector meson mass, and $W$ the energy of the $\gamma^{*}-A$ collision, a target proton can also be considered. Indeed in that case, since partons with an energy fraction as small as $x$ are probed in the target wave function, the dipole will scatter off large gluon densities generated by the QCD evolution.

In $\mathrm{e}+\mathrm{p}$ collisions, the cross-section is maximal at minimum momentum transfer with exclusive production (or coherent diffraction) dominating. As the transfer of momentum gets larger, the role of incoherent diffraction increases and eventually it becomes dominant, typically for momenta larger that the inverse target size; the elastic contribution decreases exponentially while the inelastic contribution decreases only as a power law. It is known that saturation models describe well the exclusive cross section [600, 898, 823, 899], while the BFKL Pomeron exchange approach works well for the target-dissociation cross-section [900, 901]. In the section on proton breakup, we show that, within the Color Glass Condensate (CGC) picture of the small-x part of the hadronic wave function, both coherent and incoherent diffraction can be described in the same framework. We also explicitly calculate both contributions to the diffractive vector meson production cross-section using the

McLerran-Venugopalan (MV) model for the CGC wave function, and discuss phenomenological consequences in the context of a future electron-ion collider [902].

Diffractive dissociation is an aspect of diffraction that changes qualitatively with nuclear targets. Indeed, the structure of incoherent diffraction eA $\rightarrow$ eXY is more complex than with a proton target, and also can teach us a lot more. In the case of a target nucleus, we expect the following qualitative changes in the $t$ dependence. First, the low- $|t|$ regime in which the nucleus scatters elastically will be dominant up to a smaller value of $|t|$ (to about $|t|=0.05 \mathrm{GeV}^{2}$ ) compared to the proton case, reflecting the bigger size of the nucleus. Then, the nucleus-dissociative regime will be made of two parts: an intermediate regime in momentum transfer up to about $0.7 \mathrm{GeV}^{2}$ where the nucleus will predominantly break up into its constituents nucleons, and a large- $|t|$ regime where the nucleons inside the nucleus will also break up, implying pion production in the $Y$ system for instance. These are only qualitative expectations, it is crucial to study this aspect of diffraction quantitatively in order to complete our understanding of the structure of nuclei. The transition from the coherent to the intermediate regime is studied in the nuclear breakup section, following Ref. 827.
Proton breakup: In diffractive vector meson production, the relevant quantity is (the photon is a right mover, the CGC a left mover, and the gauge is $\mathcal{A}^{+}=0$ ):

$$
\begin{equation*}
T_{\mathbf{x y}}\left[\mathcal{A}^{-}\right]=1-\frac{1}{N_{c}} \operatorname{Tr}\left(U_{\mathbf{y}}^{\dagger} U_{\mathbf{x}}\right), \quad \text { with } U_{\mathbf{x}}\left[\mathcal{A}^{-}\right]=\mathcal{P} \exp \left(i g_{S} \int d z^{+} T^{c} \mathcal{A}_{c}^{-}\left(z^{+}, \mathbf{x}\right)\right) \tag{5.88}
\end{equation*}
$$

In terms of this object, the differential cross sections for a transversely ( T ) or longitudinally (L) polarized photon are given by (with $t=-q_{\perp}^{2}$ the momentum transfer squared)

$$
\begin{equation*}
\left.\frac{d \sigma_{T, L}}{d t}=\left.\frac{1}{4 \pi}\langle | \int d z d^{2} x d^{2} y e^{i q_{\perp} \cdot(z \mathbf{x}+(1-z) \mathbf{y})} \Psi_{T, L}(z, \mathbf{x}-\mathbf{y}) T_{\mathbf{x y}}\right|^{2}\right\rangle_{x} \tag{5.89}
\end{equation*}
$$

where $2 \Psi_{T}=\Psi_{V \mid \gamma}^{++}+\Psi_{V \mid \gamma}^{--}$and $\Psi_{L}=\Psi_{V \mid \gamma}^{00}$ with

$$
\begin{equation*}
\Psi_{V \mid \gamma}^{\lambda^{\prime} \lambda}(z, \mathbf{r})=\sum_{h \bar{h}}\left[\phi_{\lambda^{\prime}}^{h \bar{h}}(z, \mathbf{r})\right]^{*} \phi_{\lambda}^{h \bar{h}}(z, \mathbf{r}), \tag{5.90}
\end{equation*}
$$

the overlap between the photon and meson wave functions. $\lambda$ and $h$ denote polarizations and helicities while $z$ is the longitudinal momentum fraction of the photon carried by the quark and $\mathbf{x}$ and $\mathbf{y}$ are the quark and antiquark positions in the transverse plane.

The target average $\langle.\rangle_{x}$ is done with the CGC wave function squared $\left|\Phi_{x}\left[\mathcal{A}^{-}\right]\right|^{2}$ :

$$
\begin{equation*}
\langle f\rangle_{x}=\int D A^{-}\left|\Phi_{x}\left[A^{-}\right]\right|^{2} f\left[A^{-}\right] \tag{5.91}
\end{equation*}
$$

If one had imposed elastic scattering on the target side to describe the exclusive process $\gamma^{*} A \rightarrow V A$, the CGC average would be at the level of the amplitude, and the two-point function $\left\langle T_{\mathrm{xy}}\right\rangle_{x}$ inside the $|.|^{2}$ in (5.89), recovering the formula often used with dipole models.

Instead, when also including the target-dissociative part, the diffractive cross section involves the 4-point correlator $\left\langle T_{\mathbf{x y}} T_{\mathbf{u v}}\right\rangle_{x}$. In order to compute it, we must specify more about the CGC wave function. We shall use the McLerran-Venugopalan (MV) model [729, 903, 730, which is a Gaussian distribution for the color charges which generate the field $\mathcal{A}$ :

$$
\begin{equation*}
\left|\Phi_{x}\left[A^{-}\right]\right|^{2}=\exp \left(-\int d^{2} x d^{2} y d z^{+} \frac{\rho_{c}\left(z^{+}, \mathbf{x}\right) \rho_{c}\left(z^{+}, \mathbf{y}\right)}{2 \mu^{2}\left(z^{+}\right)}\right) \tag{5.92}
\end{equation*}
$$

where the color charge $\rho_{c}$ and the field $\mathcal{A}_{c}^{-}$obey the Yang-Mills equation $-\nabla^{2} \mathcal{A}_{c}^{-}\left(z^{+}, \mathbf{x}\right)=$ $g_{S} \rho_{c}\left(z^{+}, \mathbf{x}\right)$. The variance of the distribution is the transverse color charge density squared along the projectile's path $\mu^{2}\left(z^{+}\right)$, with

$$
\begin{equation*}
\left\langle\rho_{c}\left(z^{+}, \mathbf{x}\right) \rho_{d}\left(z^{\prime+}, \mathbf{y}\right)\right\rangle=\delta_{c d} \delta\left(z^{+}-z^{\prime+}\right) \delta^{(2)}(\mathbf{x}-\mathbf{y}) \mu^{2}\left(z^{+}\right) . \tag{5.93}
\end{equation*}
$$

The only parameter is the saturation momentum $Q_{s}$, with $Q_{s}^{2}$ proportional to the integrated color density squared. Note that there is no $x$ dependence in the MV model, it should be considered as an initial condition to the small- $x$ evolution.

The MV distribution is a Gaussian distribution, therefore one can compute any target average by expanding the Wilson lines in powers of $g_{S} \mathcal{A}_{c}^{-}$(see (5.88)), and then use Wick's theorem [904, 905]. The results for the 4 -point function $\left\langle T_{\mathbf{x y}} T_{\mathbf{u v}}\right\rangle$ are given in 906]. We note that, in the large $-N_{c}$ limit, one has $\left\langle T_{\mathbf{x y}} T_{\mathbf{u v}}\right\rangle=\left\langle T_{\mathbf{x y}}\right\rangle\left\langle T_{\mathbf{u v}}\right\rangle$, which means that at small $-x$, the target-dissociative part of the diffractive cross-section in suppressed at large $N_{c}$, compared to the exclusive part.

The numerical results presented below are obtained with the $x$ evolution of the saturation scale modeled as in [83]: $Q_{s}(x)=\left(x_{0} / x\right)^{\lambda / 2} \mathrm{GeV}$, with $\lambda=0.277$ and $x_{0}=4.110^{-5}$ for the case of a target proton. The collinear logarithm of $Q_{s}$ is neglected, which corresponds to exact geometric scaling [752, 907, 873]: $F(x, \mathbf{r})=F\left[\mathbf{r}^{2} Q_{s}^{2}(x)\right]$. As an illustration, the resulting cross-section for diffractive $\mathrm{J} / \Psi$ production is displayed in Fig. 5.40, and separated into its coherent and incoherent contributions. The light-cone Gaussian J/ $\Psi$ wave function [908, 909 has been used in (5.90). At small values of $|t|$ where coherent diffraction dominates, our results are in agreement with HERA data 620] (one can get a better agreement with more realistic saturation models [600, 898, 823, 899, but this is not our point). Our model indicates that for $|t|>0.7 \mathrm{GeV}^{2}$ or so (this value slightly decreases when $Q^{2}$ increases), incoherent diffraction starts to dominate. This may be the reason why the data on exclusive production stop: there is too much proton-dissociative 'background'. We observe that this part of the cross-section decreases as a power law with $|t|$, rather than exponentially as the exclusive part does.

The model discussed in this work is well adapted to describe the low- and large- $|t|$ regimes in the case of scattering off a nucleus, but not the intermediate


Figure 5.40. Diffractive $J / \Psi$ production in DIS at HERA for $W=90 \mathrm{GeV}$ and different $Q^{2}$ values. regime since the constituent nucleons are absent from the description. This problem has been addressed in a complementary setup in the case of inclusive diffraction off nuclei [826, 825], and the coherent diffraction regime was found to be dominant up to about $|t|=0.05 \mathrm{GeV}^{2}$. The vector meson production case will be addressed next. While in the proton case, both exclusive and diffractive processes can be measured, it is likely that at a future electron-ion collider, the exclusive cross section cannot
be extracted: when the momentum transfer is small enough for the nucleus to stay intact, then it will escape too close to the beam to be detectable. Therefore the diffractive physics program will rely on our understanding of incoherent diffraction.
Nuclear breakup into its constituent nucleons: To simplify our calculation, we will here use a factorized impact parameter profile for the dipole cross section in a proton

$$
\begin{equation*}
\frac{\mathrm{d} \sigma_{\mathrm{dip}}^{\mathrm{p}}}{\mathrm{~d}^{2} \mathbf{b}_{T}}\left(\mathbf{b}_{T}, \mathbf{r}_{T}, x\right)=2\left(1-S_{p}\left(\mathbf{r}_{T}, \mathbf{b}_{T}, x\right)\right)=2 T_{p}\left(\mathbf{b}_{T}\right) \mathcal{N}(r, x) \tag{5.94}
\end{equation*}
$$

where $T_{p}$ is a Gaussian profile $T_{p}\left(\mathbf{b}_{T}\right)=\exp \left(-b^{2} / 2 B_{p}\right)$. In the following we shall consider two dipole cross section parametrizations, the IIM model [84, 910, 876, for which we take take $B_{p}=5.59 \mathrm{GeV}^{-2}$, and a factorized approximation of the IPsat parametrization 600, 823, for which $B_{p}=4.0 \mathrm{GeV}^{2}$. See 827] for a discussion of the origin of these values in different fits.

To extend the dipole cross section from protons to nuclei, we will take the independent scattering approximation that is usually used in Glauber theory and write the $S$-matrix as

$$
\begin{equation*}
S_{A}\left(\mathbf{r}_{T}, \mathbf{b}_{T}, x\right)=\prod_{i=1}^{A} S_{p}\left(\mathbf{r}_{T}, \mathbf{b}_{T}-\mathbf{b}_{T i}, x\right) \tag{5.95}
\end{equation*}
$$

Here $\mathbf{b}_{T i}$ are the nucleon coordinates. This independent scattering assumption is natural in IPsat-like parametrizations or the MV-model, where $r=\left|\mathbf{r}_{T}\right|, S\left(\mathbf{r}_{T}\right) \sim$ $e^{-r^{2} Q_{\mathrm{s}}{ }^{2} / 4}$ with a saturation scale $Q_{\mathrm{s}}{ }^{2}$ proportional to the nuclear thickness $T_{A}(b)$. High energy evolution, however, introduces an anomalous dimension that leads, in the nuclear case, to what could be called leading twist shadowing. With an anomalous dimension $S \sim e^{-\left(Q_{\mathrm{s}} r\right)^{2 \gamma}}$ with $\gamma \neq 1$, a proportionality $Q_{\mathrm{s}}{ }^{2} \sim T_{A}(b)$ is not equivalent to Eq. (5.95). A solution to this problem (see also the more detailed discussion in [825]) would require a realistic impact parameter dependent solution to the BK [770, 741, 747] equation which is not yet available. We point the reader to Ref. 872, for example, for a discussion of the difficulties. These are related to the long distance Coulomb tails that, physically, are regulated at the confinement length scale that is not enforced in


Figure 5.41. The quasielastic and coherent diffractive $J / \Psi$ cross sections in gold nuclei at $Q^{2}=0$ and $x_{\mathbb{P}}=0.001$. The IPsat and IIM parametrizations are shown. We also show the result for the linearized "IPnonsat" version (used e.g. in Ref. 911) where the incoherent cross section is explicitly $A$ times that of the proton. Our approximation (5.97) is not valid for small $|t|$ and has been left out of the plot. a first principles weak coupling calculation.

The average over the positions of the nucleon in the nucleus was given in eq. (5.66). The expectation valuedefined there is equivalent to the average over nucleon configurations in a Monte Carlo Glauber calculation. We are assuming that the positions $\mathbf{b}_{T i}$ are independent, i.e. neglecting nuclear correlations that would be a subject of interest in their own right (see e.g. [912]). The coherent cross section is obtained by averaging the amplitude before
squaring it, $\left|\langle\mathcal{A}\rangle_{\mathrm{N}}\right|^{2}$, and the incoherent one is the variance $\left.\left.\langle | \mathcal{A}\right|^{2}\right\rangle_{\mathrm{N}}-\left|\langle\mathcal{A}\rangle_{\mathrm{N}}\right|^{2}$ that measures the fluctuations of the gluon density inside the nucleus. Because $\langle\mathcal{A}\rangle_{\mathrm{N}}$ is a very smooth function of $\mathbf{b}_{T}$, its Fourier transform vanishes rapidly for $\Delta \gtrsim 1 / R_{A}$. Therefore, at large $\Delta$, the quasielastic cross section is almost purely incoherent.

The cross section for quasielastic vector meson production is now expressed in terms of the dipole scattering amplitude as

$$
\begin{align*}
& \frac{\mathrm{d} \sigma^{\gamma^{*} A \rightarrow V A^{*}}}{\mathrm{~d} t}=\frac{R_{g}^{2}\left(1+\beta^{2}\right)}{16 \pi} \int \frac{\mathrm{~d} z}{4 \pi} \frac{\mathrm{~d} z^{\prime}}{4 \pi} \mathrm{~d}^{2} \mathbf{r}_{T} \mathrm{~d}^{2} \mathbf{r}_{T}^{\prime} \\
&  \tag{5.96}\\
& \left.\quad \times\left.\left[\Psi_{V}^{*} \Psi\right](r, z, Q)\left[\Psi_{V}^{*} \Psi\right]\left(r^{\prime}, z^{\prime}, Q\right)\langle | \mathcal{A}_{q \bar{q}}\right|^{2}\left(x_{\mathbb{P}}, r, r^{\prime}, \boldsymbol{\Delta}_{T}\right)\right\rangle_{\mathrm{N}}
\end{align*}
$$

where we have applied corrections for the skewedness, $R_{g}$, and the real part of the scattering amplitude (see e.g. 824) We now average the square of the dipole scattering amplitude over the nucleon coordinates, using the assumptions of Eqs. (5.95) and (5.94) and taking the large $A$ limit. We are additionally assuming that $T_{A}$ is a smooth function on the distance scale defined by $B_{p}$. Averaging the square of the amplitude gives the total quasi-elastic contribution.

Note that Eqs. (5.95) and (5.94) have enabled us to write the leading contributions as proportional to the (Gaussian) proton impact parameter profile, which can then be Fourier-transformed analytically. Giving up either of these approximations would force us to numerically Fourier-transform the "lumpy" $b$-dependence corresponding to a fixed configuration of the nucleon positions. Keeping only the terms that contribute at large $|t| \gg 1 / R_{A}^{2}$ leaves us with the expression

$$
\begin{align*}
\left|\mathcal{A}_{q \bar{q}}\right|^{2}\left(x_{\mathbb{P}}, r, r^{\prime}, \boldsymbol{\Delta}_{T}\right)=16 & \pi^{2} B_{p}^{2} A \int \\
& \quad \mathrm{~d}^{2} \mathbf{b}_{T}  \tag{5.97}\\
& \times e^{-B_{p} \boldsymbol{\Delta}_{T}^{2}} e^{-2 \pi B_{p}(A-1) T_{A}(b)\left[\mathcal{N}(r)+\mathcal{N}\left(r^{\prime}\right)\right]} \mathcal{N}(r) \mathcal{N}\left(r^{\prime}\right) T_{A}(b) .
\end{align*}
$$

Equation (5.97) has a very clear interpretation. The squared amplitude is proportional to $A$ times the squared amplitude for scattering off a proton, corresponding to the dipole scattering independently off the nucleons in a nucleus. This sum of independent scatterings is then multiplied by a nuclear attenuation factor which accounts for the requirement that the dipole must not scatter inelastically off the other $A-1$ nucleons in the target (otherwise the interaction would not be diffractive). Note that factor $4 \pi B_{p} \mathcal{N}\left(r, x_{\mathbb{P}}\right)=\sigma_{p}\left(r, x_{\mathbb{P}}\right)$ is the proton-dipole cross section for a dipole of size $r$. Thus this attenuation corresponds to the probability of a dipole with a cross section which is the average of dipoles with $r$ and $r^{\prime}$ to pass though the nucleus. A similar expression can be found in Ref. 913 for example.

The coherent cross section in our approximation is given by

$$
\begin{equation*}
\frac{\mathrm{d} \sigma^{\gamma^{*} A \rightarrow V A}}{\mathrm{~d} t}=\frac{R_{g}^{2}\left(1+\beta^{2}\right)}{16 \pi}\left|\left\langle\mathcal{A}\left(x_{\mathbb{P}}, Q^{2}, \boldsymbol{\Delta}_{T}\right)\right\rangle_{\mathrm{N}}\right|^{2} \tag{5.98}
\end{equation*}
$$

where in the large $A$ and smooth nucleus limit the amplitude is

$$
\begin{equation*}
\left\langle\mathcal{A}\left(x_{\mathbb{P}}, Q^{2}, \boldsymbol{\Delta}_{T}\right)\right\rangle_{\mathrm{N}}=\int \frac{\mathrm{d} z}{4 \pi} \mathrm{~d}^{2} \mathbf{r}_{T} \mathrm{~d}^{2} \mathbf{b}_{T} e^{-i \mathbf{b}_{T} \cdot \boldsymbol{\Delta}_{T}}\left[\Psi_{V}^{*} \Psi\right]\left(r, Q^{2}\right) 2\left[1-e^{-2 \pi B_{p} A T_{A}(b) \mathcal{N}\left(r, x_{\mathbb{P}}\right)}\right] \tag{5.99}
\end{equation*}
$$

Figure 5.41summarizes the $t$-dependence of the quasielastic and coherent cross sections. Also shown is the approximation used in [911] where nonlinear effects are left out. The most
striking result is the large suppression by a factor of $\sim 3$ of the incoherent cross section due to nonlinear effects. The incoherent and coherent curves cross saround $|t| \approx 0.05 \mathrm{GeV}^{2}$, as anticipated. With a very good detection of the nuclear breakup events, the first, even the second, diffractive dips in the coherent cross section could be measurable at the EIC, providing detailed information about the average spatial distribution of gluons inside the nucleus. For understanding the initial conditions of ultra-relativistic heavy-ion collisions what has turned out to be equally important are the fluctuations in the gluon density, which are directly measured by the incoherent part of the spectrum.

## Electroproduction of $J / \Psi$

## Boris Z. Kopeliovich

Proton target: The diffractive electro-production of charmonia and the charmoniumnucleon elastic scattering are closely related. The amplitudes of diffractive electro-production of a charmonium and elastic charmonium-proton scattering in the dipole approach have the form,

$$
\begin{align*}
\mathcal{M}_{\gamma^{*} p}\left(s, Q^{2}\right) & =\sum_{\mu, \bar{\mu}} \int_{0}^{1} d \alpha \int d^{2} r_{T} \Phi_{\Psi}^{*(\mu, \bar{\mu})}\left(\alpha, \vec{r}_{T}\right) \sigma_{q \bar{q}}\left(r_{T}, s\right) \Phi_{\gamma^{*}}^{(\mu, \bar{\mu})}\left(\alpha, \vec{r}_{T}, Q^{2}\right) ;  \tag{5.100}\\
\mathcal{M}_{\Psi p}(s) & =\sum_{\mu, \bar{\mu}} \int_{0}^{1} d \alpha \int d^{2} r_{T} \Phi_{\Psi}^{*(\mu, \bar{\mu})}\left(\alpha, \vec{r}_{T}\right) \sigma_{q \bar{q}}\left(r_{T}, s\right) \Phi_{\Psi}^{(\mu, \bar{\mu})}\left(\alpha, \vec{r}_{T}\right) \tag{5.101}
\end{align*}
$$

Here, $\mu$ and $\bar{\mu}$ are the spin indices of the $c$ and $\bar{c}$ quarks, $Q^{2}$ is the photon virtuality, $\Phi_{\gamma^{*}}\left(\alpha, r_{T}, Q^{2}\right)$ is the light-cone distribution function of the photon for a $c \bar{c}$ fluctuation of separation $r_{T}$ and relative fraction $\alpha$ of the photon light-cone momentum carried by $c$ or $\bar{c}$. Correspondingly, $\Phi_{\Psi}\left(\alpha, \vec{r}_{T}\right)$ is the light-cone wave function of $J / \Psi$, or $\Psi^{\prime}$, or $\chi$.

The wave functions of charmonia are calculated in 914 solving the Schrödinger equation with four realistic potentials, which are labelled as COR [915], BT [916], LOG [917], and POW [918. Then one should make a Lorentz boost from the charmonium rest frame to the infinite momentum frame, and to switch from 3-dimensional coordinates to the light-cone variables, $p_{T}$ and $\alpha$, which are the $c$-quark transverse and fractional longitudinal momenta respectively. This was done in 914 using the popular prescription 919 .

The important ingredient of the calculations performed in 914 (compare with [920) is the Melosh spin rotation 921 which relates the 2-dimensional spinors $\chi_{c}$ and $\chi_{\bar{c}}$, describing $c$ and $\bar{c}$ in the infinite momentum frame, to the spinors $\bar{\chi}_{c}$ and $\bar{\chi}_{\bar{c}}$ in the rest frame:

$$
\begin{equation*}
\bar{\chi}_{\mathbf{c}}=\widehat{\mathbf{R}}\left(\alpha, \tilde{\mathbf{p}}_{\mathbf{T}}\right) \chi_{\mathbf{c}}, \quad \bar{\chi}_{\overline{\mathbf{c}}}=\widehat{\mathbf{R}}\left(\mathbf{1}-\alpha,-\tilde{\mathbf{p}}_{\mathbf{T}}\right) \chi_{\overline{\mathbf{c}}}, \tag{5.102}
\end{equation*}
$$

where the matrix $R\left(\alpha, \vec{p}_{T}\right)$ has the form:

$$
\begin{equation*}
\widehat{R}\left(\alpha, \vec{p}_{T}\right)=\frac{m_{c}+\alpha M-i[\vec{\sigma} \times \vec{n}] \vec{p}_{T}}{\sqrt{\left(m_{c}+\alpha M\right)^{2}+p_{T}^{2}}} . \tag{5.103}
\end{equation*}
$$

Since the $c \bar{c}$ pair is in $S$-wave, the spatial and spin dependences in the wave function factorize, and one arrives at the following light cone wave function of the $c \bar{c}$ in the infinite momentum frame

$$
\begin{equation*}
\Phi_{\psi}^{(\mu, \bar{\mu})}\left(\alpha, \vec{p}_{T}\right)=U^{(\mu, \bar{\mu})}\left(\alpha, \vec{p}_{T}\right) \cdot \Phi_{\psi}\left(\alpha, \vec{p}_{T}\right), \tag{5.104}
\end{equation*}
$$

where

$$
\begin{equation*}
U^{(\mu, \bar{\mu})}\left(\alpha, \vec{p}_{T}\right)=\chi_{c}^{\mu \dagger} \widehat{R}^{\dagger}\left(\alpha, \vec{p}_{T}\right) \vec{\sigma} \cdot \vec{e}_{\psi} \sigma_{y} \widehat{R}^{*}\left(1-\alpha,-\vec{p}_{T}\right) \sigma_{y}^{-1} \widetilde{\chi}_{\bar{c}}^{\bar{c}} \tag{5.105}
\end{equation*}
$$

Now we can determine the light-cone wave function in the mixed longitudinal momentum - transverse coordinate representation:

$$
\begin{equation*}
\Phi_{\psi}^{(\mu, \bar{\mu})}\left(\alpha, \vec{r}_{T}\right)=\frac{1}{2 \pi} \int d^{2} p_{T} e^{-i \vec{p}_{T} \vec{r}_{T}} \Phi_{\psi}^{(\mu, \bar{\mu})}\left(\alpha, \vec{p}_{T}\right) \tag{5.106}
\end{equation*}
$$

With this wave function and with the standard distribution functions of the photon one can calculate the amplitudes in (5.100)-(5.101) and predict the cross section of $J / \Psi$ photoproduction on a proton. The results for the energy dependence are compared with HERA data (see references in (914) in Fig. 5.42, The calculation was performed in 914 with two parametrizations of the dipole cross section labelled as GBW [788] and KST [795].

We see that only BP and LOG potentials describe the data well, which, however, are not sensitive to the choice of the phenomenological dipole cross section. The $Q^{2}$ dependence of the cross section is


Figure 5.42. Integrated cross section for elastic photoproduction $\gamma p \rightarrow J / \Psi p$ with real photons ( $Q^{2}=0$ ) as a function of the energy calculated with GBW and KST dipole cross sections and for four potentials to generate $J / \Psi$ wave functions. compared to HERA data (see references in [914]) in Fig. [5.43 (left) for the LOG and BT potentials. It turns out that the effects of Melosh spin rotation have a gross impact on the cross section of elastic photoproduction $\gamma p \rightarrow J / \Psi(\psi) p$. It increases the photoproduction cross section by about $50 \%$. These effects have even more dramatic impact on the $\psi^{\prime}$, increasing the photoproduction cross section by a factor of 2-3 and eliminating the large discrepancy with data observed previously 920 .

Eventually, we are in a position to predict the charmonium-proton total cross section, which is impossible to extract directly from photoproduction data, either on protons, or nuclear targets. Indeed, neither vector dominance [922], nor Glauber model 923] can be used for data analysis. We believe that the only way is to predict the charmonium cross section within a model, which successfully describe data on photoproduction in a parameter free way. Our predictions for the energy dependent charmonium-proton total cross section are depicted in Fig. 5.43 (right) for $J / \Psi$ and $\Psi^{\prime}$.

Nuclear targets: Charmonium photoproduction on nuclei is controlled by two length scales.

$$
\begin{equation*}
l_{c}=\frac{2 \nu}{M_{c \bar{c}}^{2}+Q^{2}} \approx \frac{2 \nu}{M_{J / \Psi}^{2}+Q^{2}} ; l_{f}=\frac{2 \nu}{M_{\Psi^{\prime}}^{2}-M_{J / \Psi}^{2}} \tag{5.107}
\end{equation*}
$$

The first one is called coherence length can be interpreted as the lifetime of a $\bar{c} c$ fluctuation in the projectile photon in the nuclear rest frame. When $l_{c}$ is short compared to the mean nucleon spacing, one can treat $\bar{c} c$ production as instantaneous, with following propagation of the $\bar{c} c$ dipole through the nucleus. In the opposite limit of $l_{c} \gg R_{A}$ the $\bar{c} c$ dipole propagates and attenuates through the whole nucleus. The second scalel $l_{f}$ is the formation length,


Figure 5.43. Left: Integrated cross section for elastic photo production as a function of the photon virtuality $Q^{2}+M_{J / \Psi}$ at energy $\sqrt{s}=90 \mathrm{GeV}$. Right: Total $J / \Psi-p$ (thick curves) and $\Psi^{\prime}-p$ (thin curves) cross sections with the GBW and KST parameterizations for the dipole cross section.
which characterizes the formation of the charmonium wave function. Indeed, the produced $\bar{c} c$ dipole has a certain size and interaction cross section, but does not have any certain mass. It might be the $J / \Psi$, or its radial excitation. To disentangle between them, takes time according to the uncertainty principle.

The cross section of charmonium photo-production on nuclei is easiest to write in the limit of long $l_{c} \gg R_{A}$. In this case, the size of the $\bar{c} c$ dipoles "frozen" by Lorentz time dilation for propagation of the dipole through the nucleus. The cross sections of incoherent (the nucleus break up to fragments) and coherent (the nucleus remains intact) production have the form [923, 924 ,

$$
\begin{array}{r}
\left.\sigma_{i n c}^{\gamma_{T, L}^{*} A}\left(s, Q^{2}\right)=\int d^{2} b T_{A}(b)\left|\langle\Psi| \sigma_{\bar{c} c}\left(r_{T}, s\right) \exp \left[-\frac{1}{2} \sigma_{\overline{c c}}\left(r_{T}, s\right) T_{A}(b)\right]\right| \Psi_{c \bar{c}}^{T, L}\right\rangle\left.\right|^{2} \\
\left.\sigma_{c o h}^{\gamma_{T, L}^{*} A}\left(s, Q^{2}\right)=\int d^{2} b\left|\langle\Psi| 1-\exp \left[-\frac{1}{2} \sigma_{\bar{c} c}\left(r_{T}, s\right) T_{A}(b)\right]\right| \Psi_{c \bar{c}}^{T, L}\right\rangle\left.\right|^{2} \tag{5.109}
\end{array}
$$

where $\Psi_{\bar{c} c}^{T, L}$ are the photon wave functions given by Eq. (5.27); $\Psi\left(\vec{r}_{T}, \alpha\right)$ is the charmonium light-cone wave function calculated in the previous section. These expressions are significantly different from the Glauber model [925] and effectively include the Gribov corrections in all orders.

We define the nuclear ratios for coherent and incoherent reactions as,

$$
\begin{equation*}
R_{\Psi}^{c o h}\left(s, Q^{2}\right)=\frac{\sigma_{c o h}^{\gamma^{*} A}\left(s, Q^{2}\right)}{A \sigma^{\gamma^{*} N}\left(s, Q^{2}\right)}, \quad R_{\Psi}^{i n c}\left(s, Q^{2}\right)=\frac{\sigma_{i n c}^{\gamma^{*} A}\left(s, Q^{2}\right)}{A \sigma^{\gamma^{*} N}\left(s, Q^{2}\right)} . \tag{5.110}
\end{equation*}
$$

These ratios, calculated with Eqs. (5.108)-(5.109) for real photoproduction of $J / \Psi$ and $\Psi^{\prime}$, are depicted as a function of energy in Fig. 5.44. For coherent production, the cross section rises with $A$ nearly as $A^{4 / 3}$, so the ratio may reach a large magnitude.

One can also predict the dependence on the momentum transfer $\vec{k}_{T}$ for the charmonium electro-production on nuclei. In the case of incoherent production, this dependence is the same as for production on free nucleons. However, in coherent production, the nuclear form factor comes into play and one has

$$
\begin{equation*}
\left.\frac{d \sigma_{c o h}^{\gamma_{T, L}^{*} A}\left(s, Q^{2}\right)}{d^{2} k_{T}}=\left|\int d^{2} b e^{i \vec{k}_{T} \cdot \vec{b}}\langle\Psi| 1-\exp \left[-\frac{1}{2} \sigma_{\bar{q} q}\left(r_{T}, s\right) T_{A}(b)\right]\right| \Psi_{c \bar{c}}^{T, L}\right\rangle\left.\right|^{2} . \tag{5.111}
\end{equation*}
$$



Figure 5.44. Ratios $R_{J / \Psi}^{c o h}, R_{J / \Psi}^{i n c}, R_{\Psi^{\prime}}^{c o h}$ and $R_{\Psi^{\prime}}^{c o h}$ for coherent and incoherent production on carbon, copper and Pbas function of $\sqrt{s}$ and at $Q^{2}=0$. The solid and dashed curves refer to the GBW and KST parameterizations respectively.

We introduce the ratios the sum of $T$ and $L$ components of Eq. (5.111) to the cross section at $Q^{2}=0$ and $k_{T}=0$,

$$
\begin{equation*}
\mathcal{R}\left(s, Q^{2}, k_{T}\right)=\frac{d \sigma_{c o h}^{\gamma^{*} A}\left(s, Q^{2}\right)}{d^{2} k_{T}} /\left.\frac{d \sigma_{c o h}^{\gamma^{*} A}\left(s, Q^{2}=0\right)}{d^{2} k_{T}}\right|_{k_{T}=0} \tag{5.112}
\end{equation*}
$$

This ratio is plotted in Fig. 5.45 as a function of $k_{T}$ at $s=4000 \mathrm{GeV}^{2}$ for different virtualities of the photon. We see that the $k_{T}$ dependences are rather similar for $J / \Psi$ and $\Psi^{\prime}$. The shape of the distribution is determined mainly by the nuclear geometry (and not by the size of the (small) charmonium). The calculated curves show the familiar diffraction pattern known from elastic scattering on nuclei.



Figure 5.45. Ratios $\mathcal{R}_{J / \Psi}$ and $\mathcal{R}_{\Psi^{\prime}}$ as functions of $k_{T}$ at $s=4000 \mathrm{GeV}^{2}$ for different values of $Q$. All curves are calculated with the GBW parameterization of the dipole cross section.

It is interesting that the effects of gluon shadowing, calculated in [924], do not affect much the shape and position of the minima in $k_{T}$ dependence of the coherent cross section. However, the cross section integrated over $k_{T}$ may be significantly affected by gluon shadowing. To see the magnitude of gluon shadowing, we introduce the ratio of the cross sections calculated with and without gluon shadowing,

$$
\begin{equation*}
S_{g}\left(s, Q^{2}\right)=\frac{\sigma_{g}^{\gamma^{*} A}\left(s, Q^{2}\right)}{\sigma \gamma^{*} A\left(s, Q^{2}\right)} . \tag{5.113}
\end{equation*}
$$

for incoherent and coherent exclusive charmonium electroproduction. The predicted effects
of gluon shadowing are depicted in Fig. 5.46.
We only plot ratios for $J / \Psi$ production, because ratios for $\Psi^{\prime}$ are practically the same. All curves are calculated with the GBW parameterization of the dipole cross section. We see that the onset of gluon shadowing happens at a c.m. energy of a few tens of GeV. This is controlled by the longitudinal nuclear form factor

$$
\begin{equation*}
F_{A}\left(q_{c}^{g}, b\right)=\frac{1}{T_{A}(b)} \int_{-\infty}^{\infty} d z \rho_{A}(b, z) e^{i q_{c} z} \tag{5.114}
\end{equation*}
$$

where the longitudinal momentum transfer $q_{c}^{g}=1 / l_{c}^{g}$. For the onset of gluon shadowing, $q_{c}^{g} R_{A} \gg 1$, one can keep only the double scattering shadowing correction,

$$
\begin{equation*}
S_{g} \approx 1-\frac{1}{4} \sigma_{e f f} \int d^{2} b T_{A}^{2}(b) F_{A}^{2}\left(q_{c}^{g}, b\right) \tag{5.115}
\end{equation*}
$$

where $\sigma_{\text {eff }}$ is the effective cross section which depends on the dynamics of interaction of the $\bar{q} q g$ fluctuation with a nucleon.

It was found in 787] that the coherence length for gluon shadowing is rather short, $l_{c}^{g} \approx\left(10 x m_{N}\right)^{-1}$, where Bjorken $x$ in our case should be an effective one, $x=\left(Q^{2}+\right.$ $\left.M_{\Psi}^{2}\right) / 2 m_{N} \nu$. The onset of shadowing according to (5.114) and (5.115) should be expected at $q_{c}^{2} \sim 3 /\left(R_{A}^{c h}\right)^{2}$ corresponding to $s_{g} \sim$ $10 m_{N} R_{A}^{c h}\left(Q^{2}+M_{\Psi}^{2}\right) / \sqrt{3}$, where $\left(R_{A}^{c h}\right)^{2}$ is the mean culated with and without gluon shadowing for incoherent and coherent square of the nuclear $J / \Psi$ production..
charge radius. This esti-
mate is in a good agreement with Fig. 5.46. Remarkably, the onset of shadowing is delayed with rising nuclear radii and $Q^{2}$. This follows directly from Eq. (5.115) and the fact that the formfactor is a steeper falling function of $R_{A}$ for heavy than for light nuclei, provided that $q_{c}^{G} R_{A} \gg 1$.

At medium energies, the effects of finite coherence length, $l_{c} \sim R_{A}$ become important. They increase the incoherent and suppress coherent cross sections of charmonium electroproduction. One can find the details of the corresponding calculations in 924 .

## Exclusive processes in $e+A$ collisions

Victor P. Gonçalves
Exclusive processes in deep inelastic scattering (DIS) have appeared as key reactions to trigger the generic mechanism of diffractive scattering. In particular, diffractive vector meson production and deeply virtual Compton scattering (DVCS) have been extensively
studied at HERA and provide a valuable probe of the QCD dynamics at high energies. The cross sections for exclusive processes in DIS are proportional to the square of the scattering amplitude, which makes them strongly sensitive to the underlying QCD dynamics.

In this contribution, we present our estimate for the coherent and incoherent cross sections for exclusive $\rho, J / \Psi$, and $\phi$ production as well as for nuclear DVCS, making use of the numerical solution of the Balitsky-Kovchegov equation including running coupling corrections in order to estimate the contribution of the saturation physics to exclusive processes (For more details and references see Refs. [926, 927).

Exclusive production: In the color dipole approach, exclusive production $\gamma^{*} A \rightarrow E Y$ $(E=\rho, \phi, J / \Psi$ or $\gamma)$ in electron-nucleus interactions at high energies $\left(l_{c} \gg R_{A}\right)$ is given by

$$
\begin{equation*}
\sigma^{c o h}\left(\gamma^{*} A \rightarrow E A\right)=\int d^{2} b\left\langle\mathcal{N}^{A}(x, r, b)\right\rangle^{2} \tag{5.116}
\end{equation*}
$$

where

$$
\begin{equation*}
\langle\mathcal{N}\rangle=\int d^{2} r \int d z \Psi_{E}^{*}(r, z) \mathcal{N}^{A}(x, r, b) \Psi_{\gamma^{*}}\left(r, z, Q^{2}\right) \tag{5.117}
\end{equation*}
$$

and $\mathcal{N}^{A}(x, r, b)$, defined in eq. (5.76), is the forward dipole-target scattering amplitude for a dipole with size $r$ and impact parameter $b$. We will assume that $\sigma_{d p}$ in eq. (5.76) is given by the bCGC saturation model or the solution of the running coupling BK equation.

On the other hand, if the nucleus scatters inelastically, i.e. breaks up $(Y=X)$, the process is called incoherent production. In this case, one sums over all final states of the target nucleus, except those that contain particle production. The $t$ slope is the same as in the case of a nucleon target. Therefore we have

$$
\begin{equation*}
\sigma^{i n c}\left(\gamma^{*} A \rightarrow E X\right)=\frac{|\mathcal{I} m \mathcal{A}(s, t=0)|^{2}}{16 \pi B_{E}} \tag{5.118}
\end{equation*}
$$

where at high energies $\left(l_{c} \gg R_{A}\right)$ :

$$
\begin{equation*}
|\mathcal{I} m \mathcal{A}|^{2}=\int d^{2} b T_{A}(b)\left|\Psi_{E}^{*}(r, z) \sigma_{d p} \exp \left[-\frac{1}{2} \sigma_{d p} T_{A}(b)\right] \Psi_{\gamma^{*}}\left(r, z, Q^{2}\right)\right|^{2} \tag{5.119}
\end{equation*}
$$

and $\sigma_{d p}$ is the dipole-proton cross section. In the incoherent case, the $q \bar{q}$ pair attenuates with a constant absorption cross section, as in the Glauber model, except that the whole exponential is averaged rather than just the cross section in the exponent. The coherent and incoherent cross sections depend differently on $t$. At small $-t\left(-t R_{A}^{2} / 3 \ll 1\right)$ coherent production dominates, with the signature being a sharp forward diffraction peak. On the other hand, incoherent production will dominate at large- $t\left(-t R_{A}^{2} / 3 \gg 1\right)$, with the $t$ dependence being to a good accuracy the same as in the production off free nucleons.

In Eqs. (5.117) and (5.119) the functions $\Psi^{\gamma}(z, r)$ and $\Psi^{E}(z, r)$ are the light-cone wavefunctions of the photon and the exclusive final state, respectively. The variable $r$ defines the relative transverse separation of the pair (dipole) and $z(1-z)$ is the longitudinal momentum fraction of the quark (antiquark). In the dipole formalism, the light-cone wavefunctions $\Psi(z, r)$ in the mixed representation $(r, z)$ are obtained through a two dimensional Fourier transform of the momentum space light-cone wavefunctions $\Psi(z, k)$. The photon wavefunctions are well known in the literature. For the meson wavefunction, we considered the Gauss-LC model. In the DVCS case, as one has a real photon in the final state, only


Figure 5.47. Energy dependence of the coherent (left) and incoherent (right) cross sections for different final states and $Q^{2}=1 \mathrm{GeV}^{2}$.
the transversely polarized overlap function contributes to the cross section. Summed over the quark helicities, for a given quark flavour $f$, it is given by,

$$
\begin{equation*}
\left(\Psi_{\gamma}^{*} \Psi\right)_{T}^{f}=\frac{N_{c} \alpha_{\mathrm{em}} e_{f}^{2}}{2 \pi^{2}}\left\{\left[z^{2}+\bar{z}^{2}\right] \varepsilon_{1} K_{1}\left(\varepsilon_{1} r\right) \varepsilon_{2} K_{1}\left(\varepsilon_{2} r\right)+m_{f}^{2} K_{0}\left(\varepsilon_{1} r\right) K_{0}\left(\varepsilon_{2} r\right)\right\} \tag{5.120}
\end{equation*}
$$

where we have defined the quantities $\varepsilon_{1,2}^{2}=z \bar{z} Q_{1,2}^{2}+m_{f}^{2}$ and $\bar{z}=(1-z)$. Accordingly, the photon virtualities are $Q_{1}^{2}=Q^{2}$ (incoming virtual photon) and $Q_{2}^{2}=0$ (outgoing real photon).
Results: In Fig. 5.47 left, we show the coherent production cross section as a function of the photon-target c.m.s energy, $W$, for a fixed photon virtuality $Q^{2}=1 \mathrm{GeV}^{2}$. Fig. 5.47 right is the exact analogue for the corresponding incoherent cross sections. Each one of the panels shows the results obtained for one specific final state. In each figure, the two upper (lower) curves show the results for a $\mathrm{Pb}(\mathrm{Ca})$ target. In all figures, the dashed (solid) lines are obtained with the bCGC (rcBK) dipole-proton cross section. At low $W$, the bCGC and rcBK production cross sections are indistinguishable from one another because the dipole cross sections tend to coincide. These latter have been tuned to fit DIS data, which are taken in this kinematical region. Another expected feature is the observed decrease of the cross sections with increasing vector meson masses, which comes from the wave functions. Differences are expected to appear at higher energies, where we enter the lower $x$ (extrapolation) region. In all cases we see that the results obtained with the rcBK cross section are larger than those obtained with the bCGC one. This is related to the fact that the numerical solutions of the BK equation tend to reach the unitarity limit later. Due to this fact, the results obtained with the rcBK dipole cross section grow faster with energy than those obtained with the bCGC one. Another feature is that the differences between bCGC and rcBK are larger for heavier vector mesons. Comparing the results shown in Fig. 5.47 we verify the dominance of the coherent production with a small contribution coming from incoherent processes.

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## Constraining the $\rho$ wavefunction

Jeffrey R. Forshaw and Ruben Sandapen

In the dipole model [735, 928, the imaginary part of the amplitude for diffractive $\rho$ production is written as [899]

$$
\begin{equation*}
\Im m \mathcal{A}_{\lambda}\left(s, t ; Q^{2}\right)=\sum_{h, \bar{h}} \int \mathrm{~d}^{2} \mathbf{r} \mathrm{~d} z \Psi_{h, \bar{h}}^{\gamma^{*}, \lambda}\left(r, z ; Q^{2}\right) \Psi_{h, \bar{h}}^{\rho, \lambda}(r, z)^{*} e^{-i z \mathbf{r} \cdot \boldsymbol{\Delta}} \mathcal{N}(x, \mathbf{r}, \boldsymbol{\Delta}) \tag{5.121}
\end{equation*}
$$

where $t=-|\boldsymbol{\Delta}|^{2}$. In a standard notation [929, 899, 898, $\Psi_{h, \bar{h}}^{\gamma^{*}, \lambda}$ and $\Psi_{h, \bar{h}}^{\rho, \lambda}$ are the light-cone wavefunctions of the photon and the $\rho$ meson respectively while $\mathcal{N}(x, \mathbf{r}, \boldsymbol{\Delta})$ is the imaginary part of the dipole-proton elastic scattering amplitude. The energy dependence of the latter is via the dimensionless variable $x$, taken here to be $x=\left(Q^{2}+4 m_{f}^{2}\right) /\left(Q^{2}+s\right)$ where $m_{f}$ is a phenomenological light quark mass 7 Setting $t=0$ in equation (5.121), we obtain the forward amplitude used in reference [929]:

$$
\begin{equation*}
\left.\Im m \mathcal{A}_{\lambda}\left(s, t ; Q^{2}\right)\right|_{t=0}=s \sum_{h, \bar{h}} \int \mathrm{~d}^{2} \mathbf{r} \mathrm{~d} z \Psi_{h, \bar{h}}^{\gamma, \lambda}\left(r, z ; Q^{2}\right) \hat{\sigma}(x, r) \Psi_{h, \bar{h}}^{\rho, \lambda}(r, z)^{*} \tag{5.122}
\end{equation*}
$$

where we have used the optical theorem to introduce the dipole cross-section $\hat{\sigma}(x, r)=$ $\mathcal{N}(x, r, \mathbf{0}) / s$. Note that since the momentum transfer $\boldsymbol{\Delta}$ is Fourier conjugate to the impact parameter $\mathbf{b}$, the dipole cross-section at a given energy is simply the $b$-integrated dipoleproton scattering amplitude:

$$
\begin{equation*}
\hat{\sigma}(x, r)=\frac{1}{s} \int \mathrm{~d}^{2} \mathbf{b} \mathcal{N}(x, r, \mathbf{b}) \tag{5.123}
\end{equation*}
$$

This dipole cross-section can be extracted from the $F_{2}$ data since

$$
\begin{equation*}
F_{2}\left(x, Q^{2}\right) \propto \int \mathrm{d}^{2} \mathbf{r} \mathrm{~d} z\left|\Psi_{\gamma^{*}}\left(r, z ; Q^{2}\right)\right|^{2} \hat{\sigma}(x, r) \tag{5.124}
\end{equation*}
$$

and the photon's light-cone wavefunctions are known in QED, at least for large $Q^{2}$. The $F_{2}$-constrained dipole cross-section can then be used to predict the imaginary part of the forward amplitude for diffractive $\rho$ production and thus the forward differential cross-section,

$$
\begin{equation*}
\left.\frac{d \sigma_{\lambda}}{d t}\right|_{t=0}=\frac{1}{16 \pi}\left(\Im m \mathcal{A}_{\lambda}(s, 0)\right)^{2}\left(1+\beta_{\lambda}^{2}\right), \tag{5.125}
\end{equation*}
$$

where $\beta_{\lambda}$ is the ratio of real to imaginary parts of the amplitude and is computed as in reference 929 . The $t$-dependence can be assumed to be the exponential dependence as suggested by experiment 930:

$$
\begin{equation*}
\frac{d \sigma_{\lambda}}{d t}=\left.\frac{d \sigma_{\lambda}}{d t}\right|_{t=0} \times \exp (-B|t|), \quad B=N\left(14.0\left(\frac{1 \mathrm{GeV}^{2}}{Q^{2}+M_{\rho}^{2}}\right)^{0.2}+1\right) \tag{5.126}
\end{equation*}
$$

with $N=0.55 \mathrm{GeV}^{-2}$. After integrating over $t$, we can compute the total cross-section $\sigma=\sigma_{L}+\epsilon \sigma_{T}$ which is measured at HERA. 8

[^281]Presently, several dipole models [931, 824, 910, 821, 823] are able to fit the current HERA $F_{2}$ data and there is evidence that the data prefer those incorporating some form of saturation [932]. We can use the $F_{2}$-constrained dipole cross-section in order to extract the $\rho$ light-cone wavefunction using the current precise HERA data [930, 680]. This has recently been performed in reference [929] using the Regge-inspired FSSat dipole model 931 and we shall report the results of this work here. In addition, we repeat the analysis using two alternative models [910, 824, 823] both based on the original Colour Glass Condensate (CGC) model [84. They differ from the original CGC model by including the contribution of charm quarks when fitting to the $F_{2}$ data. Furthermore in one of them 910, 824, the anomalous dimension $\gamma_{s}$ is treated as an additional free parameter instead of being fixed to its LO BFKL value of 0.63 . We shall refer to these models as CGC[0.74] and CGC[0.63] models where the number in the square brackets stands for the fitted and fixed value of the anomalous dimension respectively. For both models, we use the set of fitted parameters given in reference [824]. All three models, i.e FSSat, CGC[0.63] and CGC[0.74] account for saturation although in a $b$ - (or equivalently $t$-) independent way. Indeed, at a given energy, the dipole cross-section is equal to the forward dipole-proton amplitude or to the $b$-integrated dipole proton amplitude given by equation (5.123). Finally, all three dipole models we consider here give a good description of the diffractive structure function data [876, 933].

## Boosted Gaussian predictions

BG fits

| Dipole model | $\chi^{2} /$ data point |
| :---: | :---: |
| FSSat | $310 / 75$ |
| CGC[0.74] | $262 / 75$ |
| CGC[0.63] | $401 / 75$ |


| Model | $\chi^{2} /$ d.o.f |
| :---: | :---: |
| FSSat [929] | $82 / 72$ |
| CGC[0.74] | $64 / 72$ |
| CGC[0.63] | $83 / 72$ |

## Improved fits

| Model | $\chi^{2} /$ d.o.f |
| :---: | :---: |
| FSSat [929] | $68 / 70$ |
| CGC[0.63] | $67 / 70$ |

Table 5.4. Left: Predictions of the $\chi^{2} /$ data point using the BG wavefunction. Center: $\chi^{2} /$ d.o.f obtained when fitting $R_{\lambda}$ and $b_{\lambda}$ to the leptonic decay width and HERA data. Right: $\chi^{2} /$ d.o.f obtained when fitting $b_{\lambda}, R_{\lambda} c_{T}, d_{T}$ the leptonic decay width and HERA data.

Fitting the HERA data: Previous work [898, 899, 824] has shown that a reasonable assumption for the scalar part of the light-cone wavefunction for the $\rho$ is of the form

$$
\begin{align*}
\phi_{\lambda}^{\mathrm{BG}}(r, z)= & \mathcal{N}_{\lambda} 4[z(1-z)]^{b_{\lambda}} \sqrt{2 \pi R_{\lambda}^{2}} \exp \left(\frac{m_{f}^{2} R_{\lambda}^{2}}{2}\right) \exp \left(-\frac{m_{f}^{2} R_{\lambda}^{2}}{8[z(1-z)]^{b_{\lambda}}}\right)  \tag{5.127}\\
& \times \exp \left(-\frac{2[z(1-z)]^{b_{\lambda}} r^{2}}{R_{\lambda}^{2}}\right)
\end{align*}
$$

and is referred to as the 'Boosted Gaussian' (BG). This wavefunction is a simplified version of that proposed originally by Nemchik, Nikolaev, Predazzi and Zakharov 934]. In the original BG wavefunction, $b_{\lambda}=1$ while the parameters $R_{\lambda}$ and $\mathcal{N}_{\lambda}$ are fixed by the leptonic decay width constraint and the wavefunction normalization conditions [929]. However, when the BG wavefunction is used in conjunction with either the FSSat model or any of the CGC models, none of them is able to give a good quantitative agreement with the current HERA $\rho$-production data. This is illustrated by the large $\chi^{2}$ values in table 5.4, the situation is

## Best fit parameters

|  | $R_{L}^{2}$ | $R_{T}^{2}$ | $b_{L}$ | $b_{T}$ | $c_{T}$ | $d_{T}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| FSSat [929] | 26.76 | 27.52 | 0.5665 | 0.7468 | 0.3317 | 1.310 |
| CGC[0.63] | 27.31 | 31.92 | 0.5522 | 0.7289 | 1.6927 | 2.1457 |
| CGC[0.74] | 26.67 | 21.30 | 0.5697 | 0.7929 | 0 | 0 |

Table 5.5. Best fit parameters for each dipole model.
considerably improved by fitting $R_{\lambda}$ and $b_{\lambda}$ to the leptonic decay width and HERA data (we fit to the same data set and with the same cuts as in reference 929).

For the FSSat and CGC[0.63] models, we can further improve the quality of the fit by allowing for additional end-point enhancement in the transverse wave-function, i.e. using a scalar wave-function of the form

$$
\begin{equation*}
\phi_{T}(r, z)=\phi_{T}^{\mathrm{BG}}(r, z) \times\left[1+c_{T} \xi^{2}+d_{T} \xi^{4}\right] \tag{5.128}
\end{equation*}
$$

where $\xi=2 z-1$. The results are shown in table 5.4.


Figure 5.48. Best fits to the HERA (left) and ZEUS (right) total cross-section data. CGC[0.74]: solid; FSSat: dotted; CGC[0.63]: dashed.

The best fits obtained with each dipole model are compared to the HERA data in figures 5.48 and 5.49, The corresponding fitted parameters are given in table 5.5 Note that we achieve a lower $\chi^{2} /$ d.o.f $=0.89$ with $\operatorname{CGC}[0.74]$ than with $\mathrm{CGC}[0.63]$ and FSS at for which we obtain $\chi^{2} /$ d.o.f $=0.96$ and $\chi^{2} /$ d.o.f $=0.97$ respectively. Compared to the FSSat and CGC[0.63] fits, note that no additional enhancement in the transverse wavefunction is required in the CGC[0.74] fit. Nevertheless the extracted wavefunction still exhibits enhancement compared to the old BG wavefunction. The extracted light-cone wavefunctions are shown in figure 5.50 left.

Distribution Amplitudes: The leading twist-2 Distribution Amplitude (DA) reads 929]:

$$
\begin{equation*}
\varphi(z, \mu) \sim\left(1-\mathrm{e}^{-\mu^{2} / \Delta(z)^{2}}\right) \mathrm{e}^{-m_{f}^{2} / \Delta(z)^{2}}[z(1-z)]^{b_{L}} \tag{5.129}
\end{equation*}
$$



Figure 5.49. Best fits to the $\sigma_{L} / \sigma_{T}$ data. The H1 data are at $W=75 \mathrm{GeV}$ while the ZEUS data are at $W=90 \mathrm{GeV}$. CGC[0.74]: solid; FSSat: dotted; CGC[0.63]: dashed.


Figure 5.50. Left and center: The longitudinal and transverse light-cone wavefunctions squared at $r=0$. (CGC[0.74]: solid; FSSat: dotted; CGC[0.63]: dashed.) Right: The extracted leading twist-2 DAs at $\mu=1 \mathrm{GeV}$ compared to the DA of reference 935 also at 1 GeV (long-dashed) and the asymptotic DA (dot-dashed).
where $\Delta(z)^{2}=8[z(1-z)]^{b_{L}} / R_{L}^{2}$. This leading twist DA is only sensitive to the longitudinal wavefunction and, as illustrated in figure 5.50 right, we expect little variation in the predictions using the different dipole models. To compare with existing theoretical predictions for the DA, we compute moments:

$$
\begin{equation*}
\left\langle\xi^{n}\right\rangle_{\mu}=\int_{0}^{1} \mathrm{~d} z \xi^{n} \varphi(z, \mu) \tag{5.130}
\end{equation*}
$$

where by convention [929] $\int_{0}^{1} \mathrm{~d} z \varphi(z, \mu)=1$. In reference 929, we noted that our DA is very slowly varying with $\mu$ for $\mu>1 \mathrm{GeV}$, i.e our parameterization neglects the perturbatively known $\mu$-dependence of the DA. This statement remains true if we use the CGC[0.63] or CGC[0.74] instead of the FSSat model.

Our results are compared with the existing predictions in table 5.6. The moments obtained with our best fit, i.e with the CGC[0.74] model, are very similar to those obtained with FSSat model or the CGC[0.63]. In all cases, the results are in very good agreement with expectations based on QCD sum rules and the lattice. Finally, in figure 5.50 right, we compare our DAs with that predicted by Ball and Braun [935], at a scale $\mu=1 \mathrm{GeV}$. The agreement is reasonable given that in reference [935], the expansion in Gegenbauer polynomials is truncated at low order, which is presumably responsible for the local minimum at $z=1 / 2$. Certainly, all 4 distributions are broader than the asymptotic prediction $\sim 6 z(1-z)$.

Conclusions: We have used the current HERA data on diffractive $\rho$ production to extract

Moments of the leading twist DA at the scale $\mu$

| Reference | Approach | Scale $\mu$ | $\left\langle\xi^{2}\right\rangle_{\mu}$ | $\left\langle\xi^{4}\right\rangle_{\mu}$ | $\left\langle\xi^{6}\right\rangle_{\mu}$ | $\left\langle\xi^{8}\right\rangle_{\mu}$ | $\left\langle\xi^{10}\right\rangle_{\mu}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| (This paper) | CGC[0.74] fit | $\sim 1 \mathrm{GeV}$ | 0.227 | 0.105 | 0.062 | 0.041 | 0.029 |
| (This paper) | CGC[0.63] fit | $\sim 1 \mathrm{GeV}$ | 0.229 | 0.107 | 0.063 | 0.042 | 0.030 |
| 929 | FSSat fit | $\sim 1 \mathrm{GeV}$ | 0.227 | 0.105 | 0.062 | 0.041 | 0.029 |
| (This paper) | Old BG prediction | $\sim 1 \mathrm{GeV}$ | 0.181 | 0.071 | 0.036 | 0.021 | 0.014 |
| 936 | GenSR | 1 GeV | $0.227(7)$ | $0.095(5)$ | $0.051(4)$ | $0.030(2)$ | $0.020(5)$ |
| 937 | SR | 1 GeV | 0.26 | 0.15 |  |  |  |
| 935 | SR | 1 GeV | $0.26(4)$ |  |  |  |  |
| 938 | SR | 1 GeV | 0.254 |  |  |  |  |
| 939 | SR | 1 GeV | $0.23 \pm_{0.02}^{0.03}$ | $0.11 \pm_{0.02}^{0.03}$ |  |  |  |
| 940 | Lattice | 2 GeV | $0.24(4)$ |  |  |  |  |
|  | $6 z(1-z)$ | $\infty$ | 0.2 | 0.086 | 0.048 | 0.030 | 0.021 |

Table 5.6. Our extracted values for $\left\langle\xi^{n}\right\rangle_{\mu}$, compared to predictions based on the QCD sum rules (SR), Generalised QCD Sum Rules (GenSR) or lattice QCD.
information on the $\rho$ light-cone wavefunction. We find that the corresponding leading twist- 2 DA is broader than the asymptotic shape and agrees very well with the expectations of QCD sum rules and the lattice. We also find that the data prefer a transverse wavefunction with end-point enhancement although the degree of such an enhancement is model-dependent.

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### 5.7 Nuclear effects across the $x-Q^{2}$ plane: quarks and gluons

## Introduction

Rodolfo Sassot, Marco Stratmann, Pia Zurita

In spite of the remarkable phenomenological success of QCD as the theory of strong interactions, a detailed understanding of the role of quark and gluon degrees of freedom in nuclear matter is still lacking and poses great challenges for the theory. Ever since the discovery that quark and gluons in bound nucleons exhibit momentum distributions different from those measured in free or loosely bound nucleons [941], the precise determination of nuclear parton distribution functions (nPDF) has attracted growing attention, driving both increasingly accurate and comprehensive nuclear structure functions measurements 942 ] and a more refined theoretical understanding of the underlying physics.

The precise knowledge of nPDFs is not only required for a deeper understanding of the mechanisms associated with nuclear binding from a QCD improved parton model perspective, but is also a crucial input for the theoretical interpretation and analyses of a wide variety of ongoing and future high energy physics experiments, such as, for instance, heavy ion collisions at BNL-RHIC [943], proton-nucleus collisions to be performed at the CERN-LHC [944, or neutrino-nucleus interactions in long baseline neutrino experiments [945. Consequently, the kinematic range and the accuracy at which nPDFs are known has evolved into a key issue in many areas of hadronic and particle physics.

The standard description of DIS processes off nuclear targets is customarily done in terms of the hard scale $Q$ set by the virtuality of the exchanged photon and a scaling variable $x_{A} \equiv Q^{2} /\left(2 p_{A} \cdot q\right)$, analogous to the Bjorken variable used in DIS off nucleons. Here, $p_{A}$ is the target nucleus momentum, and, consequently, $x_{A}$ is kinematically restricted to $0<x_{A}<1$, just like the standard Bjorken variable. Alternatively, one can define another scaling variable $x_{B} \equiv A x_{A}$, where $A$ is the number of the nucleons in the nucleus. Under the assumption that the nucleus momentum $p_{A}$ is evenly distributed between the nucleons $p_{N}=p_{A} / A$, this variable resembles the Bjorken variable corresponding to the scattering off free nucleons, $x_{B} \equiv Q^{2} /\left(2 p_{N} \cdot q\right)$. However, in the context of nuclear scattering, it spans the interval $0<x_{B}<A$ by definition, reflecting the fact that a parton may in principle carry more than the average nucleon momentum.

In a naive picture, parton distributions in a nucleus are simply given by the incoherent sum of the parton distributions in the $Z$ protons and $(A-Z)$ neutrons that constitute the nucleus. In that case, the ratios between the structure functions or cross sections of two iso-scalar nuclei (with the same proportion of protons and neutrons, such as carbon and deuteron) should be just proportional to the ratio of their respective number of nucleons (or to unity if we normalize the structure functions by the number of nucleons $A$ ).

If we take into account Fermi motion effects, one would expect that in the larger nuclei, the cross section extends up to larger $x_{B}$, so the rates should typically grow to larger than unity at high $x_{B}$. What the EMC experiment found was that in addition to this motion effect, there was a significant and quite unexpected drop in the rates between approximately $x_{B} \approx 0.3$ and $x_{B} \approx 0.7$. In fig, 5.51, we show a precise measurement that illustrates both effects. which was recently performed at JLab [946 Later on, it was found that the situation was even worse for the naive picture outlined above, because at lower $x_{B}$ values, the rates showed non-trivial patterns of suppression and enhancement. These effects are called shadowing and anti-shadowing, respectively. The phenomenon has been measured at


Figure 5.51. Left: EMC effect and Fermi motion as measured at JLab 946. Right: The experimental results of Ref. 947] are illustrated for a gold target. The solid line is the result from Ref. [948] for the usual EMC effect and the dashed and dashed-dotted lines are respectively the EMC effects in the $F_{2}^{W^{+}}$and $F_{2}^{W^{-}}$structure functions. In both panels, $x \equiv x_{B}$ as defined in the text.
different $Q^{2}$ and persists at higher $Q^{2}$ but with a dependence specific for each $x_{B}$ region.
After more than 30 years of experimental and theoretical studies, a standard picture of nuclear modifications of structure functions and parton densities has not yet emerged. This is a clear target for detailed studies at the EIC, which have a large potential to qualitatively improve the current situation.

## The EMC effect at an EIC

Ian C. Cloët

The EMC effect has an immediate parton model interpretation, which is that the valence quarks in nuclei carry a smaller momentum fraction than the valence quarks in a free nucleon. There have been numerous attempts to explain the EMC effect, for example nuclear structure 949, nuclear pion enhancement [950, dynamical rescaling and inter-nucleon color conductivity [951, 952, 953], point like configurations [954] and the medium modifications to the bound nucleons [955, 956, 957, 958]. However, after more than a quarter of a century since the original EMC experiment, there is still no universally accepted explanation of the EMC effect. Therefore, it appears likely that to gain a deeper insight into the origins of the EMC effect we require new experimental information that is not accessed in traditional DIS.

An electron ion collier (EIC) provides excellent opportunities to access different aspects of the EMC effect, which are not as accessible with traditional fixed target experiments. A standout example is $W$-production via the DIS processes

$$
\begin{aligned}
& \ell^{-}+A \longrightarrow W^{-}+\nu_{\ell}+A \longrightarrow \nu_{\ell}+X, \\
& \ell^{+}+A \longrightarrow W^{+}+\bar{\nu}_{\ell}+A \longrightarrow \bar{\nu}_{\ell}+X .
\end{aligned}
$$

The extraction of the target structure functions from these reactions is possible at an EIC because of the unique ability to reconstruct the final state and therefore avoid the need to directly determine the outgoing momentum of the neutrino or anti-neutrino. The parton model expressions for the $F_{2}$ structure functions that characterize these processes are [959]

$$
\begin{align*}
& F_{2 A}^{W^{+}}(x)=\bar{u}_{A}(x)+d_{A}(x)+s_{A}(x)+\bar{c}_{A}(x),  \tag{5.131}\\
& F_{2 A}^{W^{-}}(x)=u_{A}(x)+\bar{d}_{A}(x)+\bar{s}_{A}(x)+c_{A}(x), \tag{5.132}
\end{align*}
$$

where $u_{A}(x), \bar{u}_{A}, \ldots$ are the various quark distributions of the target. In the valence quark region these $W^{ \pm}$structure functions are completely dominated by quark distributions of a single flavour, and hence a measurement of these structure functions provides direct access to the flavour decomposition of the nuclear parton distributions functions in this region. The flavour dependence of the EMC effect can then be determined, which will provide extremely important new information on the nature of this important phenomena.

The EMC effect ratio can be defined as

$$
\begin{equation*}
R^{i}=\frac{F_{2 A}^{i}}{Z F_{2 p}^{i}+N F_{2 n}^{i}}, \quad \text { where } \quad i \in \gamma, W^{ \pm} \tag{5.133}
\end{equation*}
$$

and $F_{2 p}^{i}, F_{2 n}^{i}, F_{2 A}^{i}$ are respectively the proton, neutron and nuclear structure functions. The atomic number of the nucleus is labelled by $Z, N$ is the neutron number. Using the nuclear quark distribution results from Ref. [948, we can construct the usual EMC effect associated with the exchange of a virtual photon and also the EMC effect in the $W^{ \pm}$ structure functions. These results are illustrate in Fig. 5.51 for an Au nucleus.

Therefore, measurements of $F_{2 A}^{W^{ \pm}}(x)$ for various nuclei, for example $\mathrm{C}, \mathrm{Fe}, \mathrm{Au}$ and Pb would provide important new information on the flavour dependence of the EMC effect, which in ref. [948 is predicted to be large for nuclei like Pb and Au . It is also claimed that a significant part of the NuTeV anomaly may also be explained by this isovector EMC effect 948 . Therefore, these measurements present an excellent opportunity for an EIC and will undoubtedly help us understand the origins of the EMC effect, which is essential if we are to ever have a QCD based description of nuclei.

## Nuclear gluons

## Hans J. Pirner

Historically, the very accurate NMC measurements of DIS on Tin and Carbon nuclei has allowed one to extract the gluon distribution from the scaling violation in $F_{2}(A)$. This has been done by Gousset and myself 960 for the first time. That analysis shows an enhancement of $10 \%$ i.e. antishadowing for $x \approx 0.1$ and the same amount of shadowing, namely also $10 \%$ at $x \approx 0.01$. A high experimental accuracy is demanded, therefore only a trend could be established. The asymptotic calculation of heavy charmonium production on nuclei is often proposed as another method to extract the nuclear gluon distribution based on the gluon-gluon fusion process. As shown in various papers by Kopeliovich this production is more complicated, especially for $J / \Psi$, because of initial and final state effects. Measurements of the gluon distribution would give an experimental window on the importance of gluonic effects in nuclear binding. Very little is known about the role of gauge fields in nuclei.

To gain insight on gluons in bound nucleons system, we have studied an abelian QED model 961 where the nucleon is replaced by an atom and the nucleus by a molecule, i.e., we have analysed the structure function of the photon in the $\mathrm{H}_{2}$-molecule and compared it with the structure function in the $H$-atom. The electron orbits of the hydrogen atoms in the molecule are polarized and modified by the electron exchange interaction leading to a suppression of photons at small $x$. At the momentum corresponding to the relative distance of the two protons, a small antishadowing peak is visible 961. In analogy, gluon antishadowing in the region $x=0.1$ may indicate the distance $\Delta r \approx 2 \mathrm{fm}$ between the centers of the nucleons which act as color sources of common gluon fields between nucleons.

A covalent binding of quarks may manifest itself as a density dependent lack of long range gluons at $x<0.1$ similarily to the deformation of the photon cloud in the hydrogen molecule. In addition, in non-Abelian QCD, one expects at small $x$ that the gluons from different nucleons overlap and merge. Both of these effects have also an interpretation in the nuclear rest frame in terms of the absorption of various partonic components in the wave function of the photon.

During the last ten years, the available data have been used to extract nuclear parton distributions and evolve them to high $Q^{2}$, as reviewed below. In a careful analysis one has to respect the large errors of the starting distribution at low $Q^{2}$ for the nuclear gluon distributions and also the larger $x$ region has to be included correctly - at least the fact that the nuclear gluon distribution [962] is more strongly affected by Fermi-motion of the nucleons than the quark distribution, since it has a stronger decrease at large $x$. Enhancement of the nuclear gluon distribution sets in already at $x=0.5$ which may be of importance for charmonium production at JLab 962 .

## Global fits of nuclear PDFs: current status

## Rodolfo Sassot, Marco Stratmann, Pia Zurita

From the point of view of perturbative $\mathrm{QCD}(\mathrm{pQCD})$, the extraction of nPDF can be performed in close analogy to what is routinely done for free nucleons: they are considered as non-perturbative inputs, to be inferred from data, whose relation to the measured observables and their energy scale dependence can be computed order by order in perturbation theory. Although one cannot discard potentially larger higher-twist or power corrections than in the case of free nucleons, or non-linear nuclear recombination effects, standard QCD factorization and universality of nPDFs are found to hold to a very good approximation in the kinematical range covered by present experiments.

At variance with PDFs for free nucleons, which, driven by the demand for increasingly precise predictions of the standard model, obtained an impressive degree of accuracy and refinement, extractions of $n P D F s$ are done at a considerably lower level of sophistication. Not only the number, variety, kinematical coverage, and precision of nuclear data are much more limited, but the precise parameterization of nPDFs is also much more involved as it depends not only on the energy scale $Q$ and the parton's momentum fraction $x$, but also on the size of the nucleus characterized by the atomic number $A$. In the following, we present a brief summary of the current status of nPDFs and outline limitations in the analyses imposed by the data available so far.

Thanks to its variable beam energy, the possibility to run with different nuclei, and the envisioned large luminosities, an EIC will add invaluable novel information on nPDFs from studies of the inclusive structure functions $F_{2, L}$. It will extend the kinematic range toward lower values of $x$ as well as higher scales of $Q$, allowing precise determination of the gluon distribution from scaling violations of $F_{2}$, permit the flavour separation of the quark sea and the study the onset of non-linear saturation effects at small $x$ (see Section 5.3), which eventually spoil the factorized pQCD approach.

Status of Nuclear Parton Densities. From the point of view of pQCD and a factorized approach, the description of nuclear DIS can be viewed as follows. In a DIS processes off a nuclear target, we also have a hard momentum scale $Q$ that allows one to factorize the measured cross section into a point-like partonic cross section and non-perturbative parton


Figure 5.52. Quality of the fit to nuclear DIS and Drell-Yan data; taken from Ref. 40.
densities, characteristic of partons seen in that nucleus. These "effective" parton densities factorize and encode all the non-perturbative information, including the details about the nuclear structure, and every mechanism, interaction, or effect we can imagine. Since the hard partonic cross sections are just the same as those appearing in the factorization for free nucleons, the nuclear parton densities will evolve with scale in the same way as ordinary parton densities. For similar reasons, the approach could be extended to higher orders. What is clearly not obvious within this line of reasoning is why, or how, one could split the non-perturbative effective nuclear parton density into a piece containing only the effects related to quarks and gluons belonging to single nucleon from those related to the nucleons bound in the nuclei. No field theoretical tool gives us a precise prescription of how to achieve this. It is important to keep in mind that even in lepton-nucleon scattering standard PDFs are not just naive probability densities; they are non-trivial, though perfectly well defined, objects which depend on the choice of factorization scheme and contain other ingredients such as gauge links.

What can be done, of course, is to follow a program of global QCD analyses completely analogous to the one carried out for PDFs, i.e., to extract the nPDFs and their $A$ dependence from data. In doing so one can explore if the basic properties of factorization and universality still hold in a nuclear environment. The first QCD extractions of nPDFs defined in this way were done at the end of the 90 's by two pioneering groups who performed leading order (LO) analyses of nuclear DIS data (EKS98, HKM01) [963, 828, 964 .

When introducing nPDFs, the usual approach was to propose a very simple relation between the parton distribution of a proton bound in the nucleus, $f_{i}^{A}$, and those for free protons $f_{i}$,

$$
\begin{equation*}
f_{i}^{A}\left(x_{B}, Q_{0}^{2}\right)=R_{i}\left(x_{B}, Q_{0}^{2}, A, Z\right) f_{i}\left(x_{B}, Q_{0}^{2}\right), \tag{5.134}
\end{equation*}
$$

in terms of a multiplicative nuclear correction factor $R_{i}\left(x_{B}, Q^{2}, A, Z\right)$, specific to a given
nucleus $(A, Z)$, parton flavor $i$, and initial energy scale $Q_{0}^{2}$. Such a description is convenient since the ratio $R_{i}\left(x_{B}, Q^{2}, A, Z\right)$ compares directly the parton densities with and without nuclear effects, and is closely related to the most common nuclear DIS observables, which are the ratios between the nuclear and deuterium structure functions. In Ref. [39] the alternative to relate nPDFs to standard PDFs by means of a convolution was introduced. The convolution approach implements straightforwardly effects related to rescalings or shifts in the parton's momentum fraction due to interactions with the nuclear medium. In addition, convolution integrals are the most natural language for parton dynamics beyond the LO and allow for the straightforward application of the Mellin transform techniques, convenient for a numerical fast and accurate computation of the scale dependence of PDFs and relevant cross section estimates.

Following the developments for standard PDFs, nPDFs analyses subsequently incorporated various improvements such as a consistent next-to-leading order (NLO) framework (nDS) [39, a thorough uncertainty analysis (HKN04 LO) 965, and periodical updates of the different sets in order to incorporate new data (EKPS07 LO) [966], up to NLO accuracy (HKN07 NLO, EPS09 NLO) [38, 40]. In the latest sets 40, 36] particular attention has been paid to the possible impact of $\mathrm{d}+\mathrm{Au}$ collision data from RHIC and neutrino DIS data on the global fits. A typical comparison to nuclear DIS and Drell-Yan data is shown in Fig. 5.52,

It is worth noticing that the inclusion of $d+A u$ data in nPDF fits, although neglecting any nuclear modifications in the hadronization process, leads to significantly larger gluon shadowing and antishadowing, as has been pointed out in [40]. The same data, however, can be described with much more moderate nuclear gluon PDFs, but including medium modified nFFs [967, see Section 5.10.


Figure 5.53. Comparison to neutrino data; taken from Ref. 968.
Regarding the impact of neutrino data, Schienbein et al. [36] claim that within their analysis it is not possible to reproduce simultaneously the trend of the data coming from electromagnetic nuclear DIS and some observables derived from neutrino DIS measurements. Of course, these conclusions are reached under rather stringent assumptions such as a very specific parameterization for nuclear effects and those implicit in the derivation of the neutrino DIS rates to deuteron, which have not been actually measured yet. On the other hand, using the EPS09 analysis and neutrino DIS data, Paukkunen and Salgado [968] find


Figure 5.54. Comparison between different sets of nPDFs from 969 .
no traces of such tension, besides some energy dependent fluctuations in the NuTeV data. A typical comparison to neutrino data is given in Fig. 5.53.

Different recent extractions of nPDFs are shown in Fig. 55.54. A general shortcoming of all present fits is that independent nuclear modification factors can be determined only for gluons, valence, and sea quarks without distinguishing different quark flavors. Also, present fixed-target data do not constrain nPDFs below about $x_{B} \simeq 0.01$, and the curves shown at smaller values of $x_{B}$ are mere extrapolations. Uncertainties on nPDFs are large, in particular for the nuclear gluon distribution. There is clearly a need for more precise data covering also the small $x_{B}$ region.

Conclusions. In the last few years, our knowledge of the way that both parton densities and fragmentation probabilities are modified in a nuclear environment have improved significantly. Different studies performed so far have clearly demonstrated that pQCD factorization and universality are extremely good approximations within the precision and kinematic range of the available data. Although the uncertainties and differences between different QCD global analysis are still large, the availability of more data for different processes, and their subsequent inclusion in the analyses will certainly help to reduce them further. Ultimately, the EIC will be required for precise quantitative studies and to explore the small $x_{B}$ regime where novel non-linear recombination and saturation phenomena are expected. A preliminary study of the capabilities of the EIC in these respects has been presented in Section 5.3 the EIC has the potential to determine gluon and quark nPDFs to a precision comparable to the nucleon PDFs down to $x \sim 10^{-3}$, and indeed to detect saturation effects as a deviation from DGLAP linear evolution.

## HKN nuclear parton distribution functions

## Shunzo Kumano

The Hirai, Kumano and Nagai (HKN) nuclear PDFs [965, 38] are determined by a global analysis of world data on charged-lepton DIS and Drell-Yan processes with nuclear targets. Since the PDFs of the nucleon are relatively well determined, it is appropriate to
parametrize the $n P D F s$ at the initial $Q_{0}^{2}=1 \mathrm{GeV}^{2}$ using Eq. (5.134) and

$$
\begin{equation*}
R_{i}\left(x_{B}, Q_{0}^{2}, A, Z\right)=1+\left(1-\frac{1}{A^{\alpha}}\right) \frac{a_{i}+b_{i} x+c_{i} x^{2}+d_{i} x^{3}}{(1-x)^{\beta_{i}}} \tag{5.135}
\end{equation*}
$$

The determined $u_{v}, \bar{q}$, and $g$ nPDFs from the HKN07 analysis [38] are shown for the calcium nucleus in Fig. 5.55 at $Q^{2}=1 \mathrm{GeV}^{2}$. LO and NLO results are shown with uncertainty bands, showing that nPDFs are determined more accurately at NLO. We obtain $\chi_{\text {min }}^{2} /$ d.o.f. $=1.35$ and 1.21 for the LO and NLO fits, respectively.

The valence-quark modifications are well determined because of accurate measurements on the $F_{2}$ ratios at medium $x$. The small- $x$ region is fixed by the baryon-number and charge conservations together with the modifications in the medium- and large- $x$ regions. The antiquark modifications are also determined well at small $x$ due to measurements on $F_{2}$ shadowing, and they are also fixed at $x \sim 0.1$ because of Fermilab Drell-Yan measurements. However, the region at $x>0.2$ is not determined at all. The E906/SeaQuest collaboration is currently measuring this medium- $x$ region, and there is also a possibility to measure this region with an experiment at J-PARC. In the near future, the uncertainty bands should be significantly reduced for the antiquark.

The gluon distribution has the largest uncertainties since it contributes to the $F_{2}$ and Drell-Yan ratios only as higher-order effects, and the $Q^{2}$ dependence of $F_{2}^{A} / F_{2}^{A^{\prime}}$ is not measured accurately on nuclear targets, which makes it difficult to pin down the gluon modifications measured by scaling violations of $F_{2}$. The small- $x$ nPDFs are dominated by huge gluon distributions, so that it is essential to determine them accurately for new discoveries by high-energy heavyion experiments. Therefore, it is important to mea-


Figure 5.55. Determined nuclear modifications in Ca 38. sure the $Q^{2}$ dependence of $F_{2}^{A} / F_{2}^{A^{\prime}}$ at EIC for determining nuclear gluon distributions.

In HKN07, the nPDFs are also investigated for the deuteron. In obtaining the "nucleonic" PDFs, deuteron data are used after crude nuclear corrections. Since the current PDFs could possibly contain nuclear effects, appropriate nuclear corrections should be applied in future for excluding such effects. Our codes for calculating the nPDFs and their uncertainties are available at the web site 970. The technical details are explained in Refs. [965, 38] and within the subroutine.

### 5.8 Color transparency

## Color transparency phenomena

B. Z. Kopeliovich

The nuclear medium is more transparent for colorless hadronic wave packets than predicted by the Glauber model. One can treat this phenomenon either in the hadronic basis as a result of Gribov's inelastic corrections [791], or in QCD as a result of color screening [780], an effect called color transparency (CT). Although the two approaches are complementary, the latter interpretation is more intuitive and straightforward. Indeed, a point-like colorless object cannot interact with external color fields, therefore its cross section vanishes as $\sigma(r) \propto r^{2}$ when $r \rightarrow 0$ [780]. When a colorless wave packet propagates through a nucleus, the fluctuations with small size have an enhanced survival probability which leads to a non-exponential attenuation $\propto 1 / L$ [780, where $L$ is the path length in nuclear matter.

Diffractive electro-production of vector mesons off nuclei is affected by shadowing and absorption which are different phenomena. Final state absorption of the produced meson exists even in the classical probabilistic approach which relates nuclear suppression to the survival probability $W(z, b)$ of the vector meson produced at the point with longitudinal coordinate $z$ and impact parameter $\vec{b}$,

$$
\begin{equation*}
W(z, b)=\exp \left[-\sigma_{i n}^{V N} \int_{z}^{\infty} d z^{\prime} \rho_{A}\left(b, z^{\prime}\right)\right] \tag{5.136}
\end{equation*}
$$

where $\rho_{A}(b, z)$ is the nuclear density and $\sigma_{i n}^{V N}$ is the inelastic $V N$ cross section. Shadowing, is also known to cause nuclear suppression. In contrast to final state absorption, it is a pure quantum-mechanical effect which results from destructive interference of the amplitudes for which the interaction takes place on different bound nucleons. It can be interpreted as a competition between the different nucleons participating in the reaction: since the total probability cannot exceed one, each participating nucleon diminishes the chances of others to contribute to the process. The interplay between absorption and shadowing is controlled by the two time scales introduced for the case of charmonium in eq. (5.107). They are defined similarly for other hadrons.

In the low-energy limit of short $l_{c}<l_{f} \ll R_{A}$ (shorter than the mean nucleon spacing $\sim 2 \mathrm{fm}$ ) only final state absorption matters. The ratio of the quasielastic $\gamma^{*} A \rightarrow V X$ and $\gamma^{*} N \rightarrow V X$ cross sections reads,

$$
\begin{equation*}
\left.R_{\text {inc }}\right|_{l_{c}, l_{f} \ll R_{A}} \equiv \frac{\sigma_{V}^{\gamma^{*} A}}{A \sigma_{V}^{\gamma^{*} N}}=\frac{1}{A} \int d^{2} b \int_{-\infty}^{\infty} d z \rho_{A}(b, z) \exp \left[-\sigma_{i n}^{V N} \int_{z}^{\infty} d z^{\prime} \rho_{A}\left(b, z^{\prime}\right)\right] \tag{5.137}
\end{equation*}
$$

In the limit of long $l_{c} \gg R_{A}$, it takes a different form; in the Glauber approximation,

$$
\begin{equation*}
\left.R_{i n c}\right|_{l_{c} \gg R_{A}}=\int d^{2} b T_{A}(b) \exp \left[-\sigma_{i n}^{V N} T_{A}(b)\right], \tag{5.138}
\end{equation*}
$$

One can see that the $V$ meson attenuates along the whole nucleus thickness in Eq. (5.138), but only along roughly half of that length in Eq. (5.137). The exact expression beyond VDM which interpolates between the two regimes (5.137) and (5.138) can be found in 925 .


Figure 5.56. Comparison of the dipolea pproach with E665 data 971 for nuclear effect in electroproduction of $\rho$-mesons. Left panel: $Q^{2}$ - dependence of nuclear transparency for lead and calcium. Solid and dashed curves show the results of using the Green function approach and the "frozen" approximation respectively. Right panel: $Q^{2}$-dependence of the total cross section ratio $R_{c o h}(A / C)=12 \sigma_{c o h} / A \sigma_{c o h}$.

The effects of color transparency lead to deviation from this expression. These effects, which can be understood as Gribov inelastic corrections lead to equation (5.108), which should be used to study the effects of color transparency.

Light-cone distribution functions for the photons and vector mesons. In what follows, we rely on the dipole description and need to know the distribution functions for the photon and vector mesons. To be self-consistent, we should use the same light-cone potential for describing both. In equation (5.30) for the Green function, we chose the real part of the potential of the $\bar{q} q$ dipole as in Refs. [795, (913). Solving Eq. (5.30) for the Green function with this potential and assuming similar spin structures for the vector mesons and photons, one can obtain an explicit formula for the vector meson light-cone wave function [913], depending on a "width" and a "quark mass" phenomenological parameters that were fitted to data in 934 .
Cross section on a proton. Now we are in a position to calculate the forward electroproduction diffractive amplitudes, which have the following form, The forward scattering amplitude $\left.\mathcal{M}_{\gamma^{*} N \rightarrow V N}^{T, L}\left(s, Q^{2}\right)\right|_{t=0}$ can be extracted from eq. (5.100) discussed previously. These amplitudes are normalized as $\left|\mathcal{M}^{T, L}\right|^{2}=16 \pi d \sigma_{N}^{T, L} /\left.d t\right|_{t=0}$. In what follows we calculate the cross sections $\sigma=\sigma^{T}+\epsilon \sigma^{L}$ assuming that the photon polarization is $\epsilon=1$.

For HERA data, the normalization of the cross section and its energy and $Q^{2}$ dependence are remarkably well reproduced, see [913]. This is important, since the absolute normalization is usually much more difficult to reproduce than nuclear effects, which we switch to in the nest section.

As a cross-check for the choice of the $\rho^{0}$ wave function, we also calculated the total $\rho^{0}$ nucleon cross section, which is usually expected to be roughly similar to the pion-nucleon cross section $\sigma_{\text {tot }}^{\pi N} \sim 25 \mathrm{mb}$. For the dipole cross section, we adopt the KST parameterization [795], which has been used above, and is designed to describe low- $Q^{2}$ data. Then, at $\nu=100 \mathrm{GeV}$, we obtain $\sigma_{t o t}^{\rho N}=27 \mathrm{mb}$ which is quite a reasonable number.
Diffractive electroproduction on nuclei. In the high energy regime of $l_{c} \gg R_{A}$ one can rely on Eq. (5.111) for incoherent electroproduction of $\rho$-mesons (with different quark mass and meson wave function). As a manifestation of color transparency, the nuclear ratio, also called nuclear transparency, $\operatorname{Tr}_{A}^{i n c} \equiv R_{\text {inc }}$ defined in (5.110), was predicted in 972 to rise as


Figure 5.57. Nuclear transparency for incoherent and coherent electroproduction of $\rho^{0}$ on nitrogen and lead as function of energy. Solid and dashed curves correspond to calculations with and without gluon shadowing, respectively. Left two panels: Incoherent production at $Q^{2}=0,1,3,5,10 \mathrm{GeV}^{2}$. Right two panels: Coherent production at $Q^{2}=0,3,10 \mathrm{GeV}^{2}$.
function of $Q^{2}$. Indeed, the mean size of the $\bar{q} q$ component of the virtual photon decreases qith $Q^{2}$, so the nucleus becomes more transparent. The results of the E665 experiment at Fermilab 971 depicted in Fig. 5.56 are in a good accord with the predicted behavior. The calculations performed in the "frozen" approximation ( $l_{c} \gg R_{A}$ ) are presented with dashed curves. The more realistic results including finiteness of $l_{c}$ and $l_{f}$ are plotted by solid curves. While the "frozen" approximation is rather accurate for incoherent production, the deviation from its expectation for coherent process at the energy of the E665 experiment is significant.

The predicted energy dependence of the nuclear ratios in incoherent and coherent $\rho$ production on nitrogen and lead are depicted in Fig. 5.57. As was expected, the nucleus becomes more opaque with energy for incoherent production. This happens because when the hadronic fluctuations of the virtual photon live longer, they propagate through the whole nucleus and attenuate more. On the other hand, in incoherent production the phase shifts between the amplitudes of $\rho$ production on different nucleons must me very small in order the nucleus remained intact. This is why the nuclear ratio depicted in the bottom part of Fig. 5.57 is so suppressed at low energies.

At high energies, such as at an EIC, gluon shadowing causes an additional nuclear suppression of $\rho$ production. This correction is calculated as was described in Sect. 5.2 and the final results are plotted in Fig. 5.57 by solid curves. As was expected, the effect of gluon shadowing is not significant.

## From color transparency to color opacity

## Mark Strikman

Color transparency (CT) phenomena play several roles. They probe both the high energy dynamics of the strong interaction and the minimal small size components of the hadrons. In the case when some of the produced particles have energies smaller than 10 GeV in the nucleus rest frame, these processes could be also used to study the space-time evolution of small wave packets - a question relevant for interpretation of heavy-ion collisions. They also provide an important link to the hard QCD black disk regime - the regime of strong absorption for the processes which at lower energies exhibit the CT regime, and determine the kinematics where factorization can be applied to generalized parton distribution studies.

The basic feature of CT is the suppression of the interaction of small size color singlet
configurations: for a dipole of transverse size $d$, perturbative QCD gives

$$
\begin{equation*}
\sigma\left(d, x_{N}\right)=\frac{\pi^{2}}{3} \alpha_{s}\left(Q_{e f f}^{2}\right) d^{2}\left[x_{N} G_{N}\left(x_{N}, Q_{e f f}^{2}\right)+2 / 3 x_{N} S_{N}\left(x_{N}, Q_{e f f}^{2}\right)\right] \tag{5.139}
\end{equation*}
$$

where $Q_{e f f}^{2} \propto 1 / d^{2}, x_{N}=Q_{e f f}^{2} / W^{2}$, and the second term is due to the contribution of quark exchanges which is important for intermediate energies 973]. There are two critical requirements for CT phenomena: squeezing, the selection of small size configurations, and freezing, the selection of high enough energies to allow the squeezed configuration to live long enough.

At high energies, one can select CT processes by selecting special final states: for example, the diffraction of a pion into two high $p_{t}$ jets, or a small initial state $\gamma_{L}^{*}$ such as in the exclusive production of mesons. QCD factorization theorems [572, 973] were proven for these processes based on the CT property of QCD. The space time picture of these processes in the nucleus rest frame is as follows: long before the target, the projectile pion or virtual photon fluctuates into a $q \bar{q}$ configuration with transverse separation $d$, which elastically scatters off the target with an amplitude which for $t=0$ is given by Eq. (5.139) (up to small corrections due to different off shellness of the $q \bar{q}$ pair in the initial and final states), followed by the transformation of the pair into two jets or a vector meson. With a slight simplification, the amplitude for dijet diffractive production can be written as

$$
\begin{equation*}
A(\pi N \rightarrow 2 \mathrm{jets}+N)\left(z, p_{t}, t=0\right) \propto \int d^{2} d \psi_{\pi}^{q \bar{q}}(d, z) \sigma_{q \bar{q}-N(A)}(d, s) e^{i p_{t} d} \tag{5.140}
\end{equation*}
$$

where $z$ is the light-cone fraction of the pion momentum carried by a quark, and $\psi_{\pi}^{q \bar{q}}(z, d) \propto$ $z(1-z)_{d \rightarrow 0}$ is the quark-antiquark Fock component of the meson light cone wave function. The presence of the plane-wave factor in the final state leads to an expectation of an earlier onset of scaling than in the case of the vector meson production, where the vector meson wave function appears instead. CT was observed in the pion diffraction into two jets [974, confirming predictions in [975. The HERA data on exclusive vector meson production are also well described.

## Investigations at an EIC

Studies at an EIC will require investigations of different exclusive meson production channels as a function of $x, Q^{2}$. In the CT limit and $-t \geq 0.1 \mathrm{GeV}^{2}$, where coherence effects are negligible, one expects

$$
\begin{equation*}
\sigma_{\gamma_{L}^{L} A \rightarrow " m e s o n " A^{*}}^{i n c o h}(t)=Z \sigma_{\gamma_{L}^{*} p \rightarrow " \text { meson" } N}(t)+N \sigma_{\gamma_{L}^{*} n \rightarrow " \text { meson" } N}(t) \tag{5.141}
\end{equation*}
$$

In EIC kinematics, the coherence length is $\gg 2 R_{A}$ so deviations from the CT prediction could be due to leading twist effects - leading twist shadowing, and higher twist effects of multiple interactions of the $q \bar{q}$ pair with the target nucleus. There are two distinctive regimes: $x \geq 0.03$ where nuclear PDFs are practically linear in A, and $x \leq 0.01$ where a significant LT shadowing of nPDFs is expected (see discussion in section 5.2).
The $x \geq 0.03$ region. Multiple interactions should reduce the cross section. At an EIC, it would be possible to perform a scan as a function of $Q^{2}$. For low $Q^{2}$ and especially for $\sigma_{T}$, one expects a hadron-like regime in which absorption is strong and $\sigma_{\gamma_{L}^{2} A \rightarrow " \text { meson" } A^{*}}^{i n c o h}(t) \propto A^{1 / 3}$. With an increase of $Q^{2}$, one expects a transition from soft dynamics with Gribov-Glauber type screening to the CT regime without significant LT gluon shadowing. In the case of $J / \psi$
production, one expects the CT regime already at low $Q^{2}$ while for the light mesons, the onset of CT can be much slower as essential transverse sizes of the $q \bar{q}$ pair decrease rather slowly with $Q^{2}$ as manifested in the slow convergence of the t-slope of $\rho$-meson production to the t-slope of $J / \psi$ production with increasing $Q^{2}$ [976].
The $x \leq 0.01$ region. In this regime, one expects large shadowing due to the LT mechanisms both for the incoherent and coherent contribution in which case 977, perturbative color opacity is given by

$$
\begin{equation*}
\frac{d \sigma_{\gamma_{L} A \rightarrow V A}}{d t} / \frac{d \sigma_{\gamma_{L} N \rightarrow V N}}{d t}=G_{A}^{2}\left(x, Q_{e f f}^{2}\right) / G_{N}^{2}\left(x, Q_{e f f}^{2}\right) \cdot F_{A}^{2}(t) \tag{5.142}
\end{equation*}
$$

where $F_{A}(t)$ is the nucleus form factor. Typical results for the expected suppression effect are given in Fig. 5.58. Note here that effective $Q^{2}$, which enters in Eq.5.142, is much smaller than $Q^{2}$ in the electro-production of light vector mesons. For example, in the case of the $\rho$ meson, $Q_{e f f}^{2} \sim 3 \mathrm{GeV}^{2}$ for $Q^{2} \sim 10 \mathrm{GeV}^{2}$. For $J / \psi$ photo-production, $Q_{e f f}^{2} \sim 3 \div 4 \mathrm{GeV}^{2}$ and grows slowly with $Q^{2}$ [978. Hence, for the top EIC energies, one expects a reduction in the coherent $J / \psi$ photo/electro production of at least a factor of two. Numerically, the LT shadowing mechanism leads to a larger screening effect for the interaction of the small dipoles than the HT dipole eikonal models (cf. [976]).

The incoherent cross section, $\sigma_{i n c o h}$, is shadowed somewhat more strongly than the coherent cross section, $\sigma_{c o h}$. The effect grows with the increasing strength of the elementary interaction. As a result, the ratio $B_{\gamma^{*} N \rightarrow " V}^{-1}{ }^{\prime \prime} N \cdot \sigma_{i n c o h} / \sigma_{\text {coh }}$ of incoherent and coherent cross sections integrated over $t$ and divided by the slope of the elementary cross section is expected to decrease slowly with decreasing $x$ at fixed $Q^{2}$ (cf. Fig. 43 in [979]). For example, for $B=4 \mathrm{GeV}^{-2}, R \equiv \sigma_{\text {incoh }} / \sigma_{c o h}$ changes from $R \approx 0.3$ in the impulse approximation limit to $R \approx 0.18$ in the regime of strong absorption (strength of dipole interaction of the order $\left.\sigma_{t o t}(\pi N)\right)$. Simultaneous measurements of coherent and incoherent diffraction will allow the testing of the underlying dynamics in greater detail.

Note that it will be feasible to measure the coherent cross section at $t \sim 0$ due to the very steep $t$ dependence of coherent peak and the ability to kill most of the incoherent diffraction experimentally. At the same time, measurements of the $t$ dependence of coherent diffraction beyond the first minimum are unlikely (except for the lightest nuclei like ${ }^{4} H e$ ) due to the dominance of processes of the nuclear excitations for $-t \geq-t_{1}$. (Measurements of very soft photons at rather large opening angles are required 980 .) Note that the cross section of inelastic diffraction with production of hadrons in the nucleus fragmentation region is comparable to that of quasi-elastic diffraction. Studies of the t-dependence of the meson production and/or hadron production in the nucleus fragmentation regionare required to separate these two processes.
Testing the onset of the black disk regime. The study of vector meson production provides a fine probe to test the onset of high density color opacity regime where the LT approximation breaks down - the black disk regime in which interactions of small dipoles with heavy nuclei become completely absorptive. In this limit, one can derive a model independent prediction for the cross section of the vector meson production [981]:

$$
\begin{equation*}
\frac{d \sigma^{\gamma_{T}^{*}}+A \rightarrow V+A}{d t}=\frac{M_{V}^{2}}{Q^{2}} \frac{d \sigma_{L}^{\gamma_{L}^{*}+A \rightarrow V+A}}{d t}=\frac{\left(2 \pi R_{A}^{2}\right)^{2}}{16 \pi} \frac{3 \Gamma_{V} M_{V}^{3}}{\alpha\left(M_{V}^{2}+Q^{2}\right)^{2}} \frac{4\left|J_{1}\left(\sqrt{-t} R_{A}\right)\right|^{2}}{-t R_{A}^{2}} \tag{5.143}
\end{equation*}
$$

where $\Gamma_{V}$ is the electronic decay width $V \rightarrow e^{+} e^{-}, \alpha$ is the fine-structure constant. Eq. (5.143) corresponds to a drastically different result: a factor of $Q^{4}$ slower $Q^{2}$ dependence of the cross section than the LT result.


Figure 5.58. Leading twist shadowing effect for coherent vector meson production off Ca and Pb . Bands reflect the range of predictions given by the FGS10_L and FGS10_H parametrizations of the gluon LT shadowing.


Figure 5.59. Examples of $2 \rightarrow 3$ processes probing (a) nucleon GPDs and large angle $\gamma^{*}(q \bar{q}) \rightarrow$ $\pi \pi(\pi \rho)$ scattering; (b) photon GPDs and large angle nucleon $(q \bar{q}) \rightarrow \pi N$ scattering, (c) nucleon $\rightarrow$ meson GPD and large angle $\gamma^{*}(q q q) \rightarrow \rightarrow \pi N$ scattering.

Other directions of studies. Recently, a number of novel processes were suggested to check the interplay between CT and color opacity phenomena as well as to use CT to understand the dynamics of various elementary processes.

1. It was demonstrated that it is possible to trace small dipoles through the center of the nucleus by selecting large $t \mathrm{VM}$ production with rapidity gap $\gamma^{*} A \rightarrow V+g a p+Y$ for $x_{g}=-t /\left(-t+M_{Y}^{2}\right) 982$.
2. It was suggested that amplitudes of high energy $2 \rightarrow 3$ branching processes: $a+b \rightarrow$ $c+d+e$, where $t=\left(p_{b}-p_{e}\right)^{2}$ is small, $t^{\prime}=\left(p_{a}-p_{c}\right)^{2}, s^{\prime}=\left(p_{c}+p_{e} d\right)^{2}$ are large, and $t^{\prime} / s^{\prime}=$ const can be written in a factorized form as a convolution of different nucleon quark GPDs and hard $2 \rightarrow 2$ amplitudes [983]. Several examples of such processes are depicted in Fig. 5.59, In the case of the ep collider one would be able to study both the nucleon GPDs and GPDs of the real (virtual photon). Also, it will be possible to study large angle $\gamma\left(\gamma^{*}\right)+(q \bar{q}) \rightarrow$ meson $_{1}+$ meson $_{2}$ and $\gamma\left(\gamma^{*}\right)+(q q q) \rightarrow$ meson + baryon reactions.
3. Embedding these processes in nuclei, for example by studying the process $\gamma+A \rightarrow$ $\pi^{+} \pi^{+} A^{*}$, will make it possible to determine at what $p_{T}$ of the pions CT sets in and hence determine minimal $p_{T}$ for which these processes could be used to study various quark GPDs. The nuclear transparency for these processes is very sensitive
to the size of the meson $\bar{q}$ configurations 984. Hence it may be possible to determine the characteristic transverse size of the $q \bar{q}$ dipole involved in the hard process using Eq. (5.139). Also, by studying the transparency as a function of $s$ for fixed $s^{\prime}, t$ and $t^{\prime}$, one could measure in great detail the rate and the pattern of the space time evolution of small $q \bar{q}$ wave packets.

### 5.9 Nuclear GPDs and TMDs

### 5.9.1 Nuclear quark and gluon GPDs

Vadim Guzey, Mark Strikman

Generalized parton distributions (GPDs) parameterize the response of hadronic targets (nucleon, nucleus) when probed by hard probes in exclusive reactions. The QCD factorization theorems state that GPDs are universal distributions that can be accessed in a wide range of hard exclusive processes: deeply virtual Compton scattering (DVCS) 624, electroproduction of mesons by longitudinal virtual photons [572], time-like Compton scattering, etc. GPDs are fundamental and rigorously-defined quantities that encode information on: (i) the distributions and correlations of partons in hadrons that is much richer than that contained in usual diagonal parton distributions and elastic form factors (in a certain sense, GPDs provide three-dimensional parton imaging), (ii) parton total angular momentum (thus, GPDs are believed to help resolve the so-called proton spin crisis), etc. For the detailed discussion of GPDs, see section 3.1 on "Imaging QCD Matter"

While what has been said above holds true for any hadronic target, nuclear GPDs are also interesting in their own right:
(i) Nuclear GPDs give access to both proton and neutron GPDs [985, 986, 987, 988, 989 . Incoherent reactions (with nuclear break-up) can be used to study quasi-free neutron GPDs 990.
(ii) Traditional nuclear effects-off-diagonal EMC effect 991, 992], nuclear shadowing and antishadowing [993, 994, 807]-have been predicted to be more prominent than in the diagonal case.
(iii) Nuclear GPDs may be a good tool to study not well-established/controversial and novel nuclear effects such as the medium modifications of bound nucleon GPDs 992, 995 and presence of non-nucleonic degrees of freedom 996].

Medium $x_{B}>0.05$
The cleanest way to study GPDs is deeply virtual Compton scattering (DVCS), $\gamma^{*}+A \rightarrow$ $\gamma+A^{\prime}$. Nuclear DVCS is more complex and versatile than that with the free proton because the nuclear target, $A$, can have various spins (the number of GPDs increases with the spin of the target) and many different final states, $A^{\prime}$, can be produced ( $A^{\prime}=A, A^{*}, A+\pi, A-1+N$, etc.). In the situation when the final nuclear state cannot be detected, one can sum over all final states $A^{\prime}$ assuming their completeness and obtain for the nuclear DVCS cross section [988]:

$$
\begin{equation*}
\sigma_{\mathrm{DVCS}}=A(A-1) \sigma_{\mathrm{DVCS}}^{\mathrm{coh}}+A \sigma_{\mathrm{DVCS}}^{N} . \tag{5.144}
\end{equation*}
$$

In this expression, the first term is the coherent-dominated contribution (without nuclear break-up or excitation) which is proportional to the nuclear form factor squared, $F_{A}^{2}$, and significant only at the small momentum transfer $t$. The second term is the incoherent contribution whose $t$ dependence is governed by that of the nucleon GPDs; this term dominates at large $t$.

Similarly to Eq. (5.144), the expressions interpolating between the coherent and incoherent regimes can also be derived for the interference between DVCS and Bethe-Heitler
(BH) amplitudes and BH cross section. For instance, the coherent-dominated contribution to the interference between DVCS and BH amplitudes scales as $Z(A-1)$ and that to the BH cross section scales as $Z(Z-1)(Z$ is the nuclear charge). Therefore, one immediately and model-independently predicts the enhancement of the ratio of the nuclear to free proton DVCS beam-spin asymmetries at small $t, A_{\mathrm{LU}}^{A} / A_{\mathrm{LU}}^{p} \sim(A-1) /(Z-1)$ [987, 988]. At large $t$, the cross section is dominated by the incoherent contribution, no nuclear enhancement is expected, and $A_{\mathrm{LU}}^{A} / A_{\mathrm{LU}}^{p} \sim 1$ (in fact, the neutron contribution somewhat suppresses the ratio and makes $A_{\mathrm{LU}}^{A} / A_{\mathrm{LU}}^{p}<1$ [989]). While the HERMES analysis of nuclear DVCS with ${ }^{4} \mathrm{He},{ }^{14} \mathrm{~N},{ }^{20} \mathrm{Ne},{ }^{84} \mathrm{Kr}$, and ${ }^{132} \mathrm{Xe}$ targets supports that $A_{\mathrm{LU}}^{A} / A_{\mathrm{LU}}^{p} \sim 1$ at large $t$ and $A$-independent at all $t$, it finds that at small $t, A_{\mathrm{LU}}^{A} / A_{\mathrm{LU}}^{p}=0.91 \pm 0.19$ [672].

Quark nuclear GPDs in the kinematic region of the off-diagonal EMC effect, $0.1<$ $x_{B}<0.3$, will be constrained with high precision by the analysis CLAS data on DVCS on ${ }^{4}$ He 997. The experiment measured purely coherent nuclear DVCS (the recoiled nucleus was detected using the BoNuS spectator tagger) and also DVCS on a quasi-free proton. The latter will probe possible nuclear medium modifications of the bound proton quark GPDs [995]. Gluon GPDs in nuclei can be accessed best in hard exclusive production of heavy vector mesons. For instance, coherent $J / \psi$ production for $x_{B}>0.1$ can be used to learn about the off-diagonal EMC effect in the gluon channel. The incoherent production of $J / \psi$ can be used to probe medium modifications of the gluon GPD of the bound nucleon.

The EIC will be the only other accelerator beside JLab 12 GeV to study GPDs in $e+A$ collisions, and will contribute considerably to their knowledge. In particular, it will access sea quark and gluon distributions, which are hard to measure at 6 GeV due to the limited $x$ and $Q^{2}$ range, and open dedicated channels like $J / \Psi$ diffreactive production.

## Small $x_{B}<0.05$ : leading twist shadowing and exclusive diffraction

The EIC will open the way to experimental measurements of nuclear GPDs at small $x_{B}$, where nuclear shadowing is known to occur for PDFs. The leading twist theory of nuclear shadowing (see section 5.2) allows one also to predict the impact parameter dependence of nuclear PDFs [807, 803, 805, 806]. The resulting impact parameter dependent nuclear PDFs, $f_{j / A}\left(x, Q^{2}, b\right)$ are the corresponding nuclear generalized parton distributions (GPDs) in the $\xi \rightarrow 0$ limit and in impact parameter space [994], $f_{j / A}\left(x, Q^{2}, b\right)=H_{A}^{j}\left(x, \xi=0, b, Q^{2}\right)$, where the latter GPD depends in general on two light-cone fractions $x$ and $\xi ; \xi$ is fixed by the external kinematics, $\xi=x_{B} /\left(2-x_{B}\right)$, where $x_{B}$ is the standard Bjorken $x$. The number of GPDs depends on the spin of the target; we shall consider only spinless targets characterized by one twist-two chirally-even GPD $H^{j}$ ( $j$ is the parton flavor).

Using the predictions of the leading twist theory of nuclear shadowing for the impact parameter dependence of nuclear PDFs (Eq. (5.33)) and the connection of these to GPDs, one can obtain the nuclear GPD $H_{A}^{j}$ at small $x$ in the $\xi=0$ limit. The final result for the GPDs in the momentum space is

$$
\begin{align*}
H_{A}^{j}(x, \xi & \left.=0, t, Q^{2}\right)=A F_{A}(t) f_{j / N}\left(x, Q^{2}\right) \\
& -\frac{A(A-1)}{2} 16 \pi \Re e\left\{\frac{(1-i \eta)^{2}}{1+\eta^{2}} \int d^{2} b e^{i \vec{\Delta}_{\perp} \cdot \vec{b}} \int_{\infty}^{\infty} d z_{1} \int_{z_{1}}^{\infty} d z_{2} \int_{x}^{0.1} d x_{\mathbb{P}} \rho_{A}\left(b, z_{1}\right)\right. \\
& \left.\times \rho_{A}\left(b, z_{2}\right) e^{i m_{N} x_{\mathbb{P}}\left(z_{1}-z_{2}\right)} e^{-\frac{A}{2}(1-i \eta) \sigma_{\text {soft }}^{j}\left(x, Q^{2}\right) \int_{z_{1}}^{z_{2}} d z^{\prime} \rho_{A}\left(b, z^{\prime}\right)} \frac{1}{x_{\mathbb{P}}} f_{j}^{D(4)}\left(\beta, Q^{2}, x_{\mathbb{P}}, t_{\min }\right)\right\}, \tag{5.145}
\end{align*}
$$



Figure 5.60. The ratio of the gluon and $\bar{u}$-quark $H_{A}^{j}(x, \xi=0, t) /\left[A F_{A}(t) f_{j / N}\left(x, Q^{2}\right)\right]$ for ${ }^{208} \mathrm{~Pb}$ as a function of $x$ for different values of $t$. All curves correspond to $Q^{2}=4 \mathrm{GeV}^{2}$ and model FGS10_H.
where the notation is the same as in eqs. (5.32) and (5.33).
Fig. 5.60 presents our predictions for the ratio $H_{A}^{j}\left(x, \xi=0, t, Q^{2}\right) /\left[A F_{A}(t) f_{j / N}\left(x, Q^{2}\right)\right]$ for ${ }^{208} \mathrm{~Pb}$ as a function of $x$ for different values of $t$. The left panel corresponds to the ratio of the $\bar{u}$-quark distributions; the right panel corresponds to the gluon distributions. All curves correspond to $Q^{2}=4 \mathrm{GeV}^{2}$ and model FGS10_H (see details in section 5.2). Since the $t$ dependence of the shadowing correction to $H_{A}^{j}(x, \xi=0, t)$ (second term in Eq. (5.145)) is somewhat slower than that of the impulse approximation (the first term), the effect of nuclear shadowing increases as $|t|$ is increased, as expected.

Experimental observables measured in hard exclusive processes such as, e.g., $\gamma^{*}+A \rightarrow$ $\gamma(J / \Psi, \rho, \ldots)+A$, probe the GPD $H_{A}^{j}\left(x, \xi, t, Q^{2}\right)$ integrated over the entire region of the light-cone variable $x, 0 \leq x \leq 1$. However, at high energies (small $\xi$ or $x_{B}$ ), the situation simplifies: the predominantly imaginary $\gamma^{*}+A \rightarrow \gamma(J / \Psi, \rho, \ldots)+A$ scattering amplitudes are expressed solely in terms of the GPDs at the $x=\xi$ cross-over line, $H_{A}^{j}\left(\xi, \xi, t, Q^{2}\right)$ (to the leading order in the strong coupling constant $\alpha_{s}$ ). In addition, it was shown in 592 that at high energies and in the leading logarithmic approximation (LLA), GPDs at an input scale $Q_{0}^{2} \sim$ few $\mathrm{GeV}^{2}$ can be approximated well by the usual parton distributions, i.e., it is safe to neglect the effect of the skewness $\xi$. Therefore, for instance, for the imaginary part of the coherent nuclear deeply virtual Compton scattering (DVCS) amplitude ( $\gamma^{*}+A \rightarrow \gamma+A$ ), we have at the leading order in $\alpha_{s}$ :

$$
\begin{align*}
\Im m \mathcal{A}_{\mathrm{DVCS}}\left(\xi, t, Q^{2}\right) & =-\pi \sum_{q} e_{q}^{2}\left[H_{A}^{q}\left(\xi, \xi, t, Q^{2}\right)+H_{A}^{\bar{q}}\left(\xi, \xi, t, Q^{2}\right)\right] \\
& \approx-\pi \sum_{q} e_{q}^{2}\left[H_{A}^{q}\left(\xi, \xi=0, t, Q^{2}\right)+H_{A}^{\bar{q}}\left(\xi, \xi=0, t, Q^{2}\right)\right] \tag{5.146}
\end{align*}
$$

where $e_{q}$ are the quark charges; $H_{A}^{q}\left(\xi, \xi=0, t, Q^{2}\right)$ are given by Eq. (5.145).
The cleanest way to access GPDs is via DVCS. At the photon level, the $\gamma^{*}+A \rightarrow \gamma+A$ cross section reads, (see, e.g., 625):

$$
\begin{equation*}
\frac{d \sigma_{\mathrm{DVCS}}}{d t}=\frac{\pi \alpha_{\mathrm{em}}^{2} x^{2}\left(1-\xi^{2}\right)}{Q^{4} \sqrt{1+\epsilon^{2}}}\left|\Im m \mathcal{A}_{\mathrm{DVCS}}\left(\xi, t, Q^{2}\right)\right|^{2} \tag{5.147}
\end{equation*}
$$

where $\alpha_{\mathrm{em}}$ is the fine-structure constant; $\epsilon^{2}=4 x^{2} m_{N}^{2} / Q^{2} ; \Im m \mathcal{A}_{\mathrm{DVCS}}$ is given by Eq. (5.146).
The DVCS process interferes and competes with the purely electromagnetic BetheHeitler ( BH ) process. The BH cross section at the photon level can be written in the


Figure 5.61. The DVCS (solid curves) and Bethe-Heitler (dot-dashed curves) cross sections for ${ }^{208} \mathrm{~Pb}$ at $Q^{2}=4 \mathrm{GeV}^{2}$. Left panel: $t$-integrated cross sections vs. $x$. The four BH curves correspond, from left to right, to $\sqrt{s}=(32,44,66,90) \mathrm{GeV}$. Middle panel: differential cross sections vs. $|t|$ at fixed $x=5 \times 10^{-3}$; the BH curve corresponds to $\sqrt{s}=32 \mathrm{GeV}$. Right panel: beam-spin asymmetry $A_{L U}$.
following form 625]:

$$
\begin{equation*}
\frac{d \sigma_{\mathrm{BH}}}{d t}=\frac{\pi \alpha_{\mathrm{em}}^{2}}{4 Q^{2} t(1+\epsilon)^{5 / 2}\left(1-y-y^{2} / 2\right)} \int_{0}^{2 \pi} \frac{d \phi}{2 \pi} \frac{1}{\mathcal{P}_{1}(\phi) \mathcal{P}_{2}(\phi)}\left|\mathcal{A}_{\mathrm{BH}}\left(\xi, t, Q^{2}, \phi\right)\right|^{2} \tag{5.148}
\end{equation*}
$$

where $y=\left(q \cdot P_{A}\right) /\left(k \cdot P_{A}\right)=Q^{2} /(x s)$ ( $k$ is the incoming lepton momentum, $q$ is the momentum of the virtual photon, $P_{A}$ is the momentum of the incoming nucleus, $s$ is the total invariant energy squared); $\phi$ is the angle between the lepton and hadron scattering planes; $\mathcal{P}_{1}(\phi)$ and $\mathcal{P}_{2}(\phi)$ are proportional to the lepton propagators; $\left|\mathcal{A}_{\mathrm{BH}}\left(\xi, t, Q^{2}\right)\right|^{2}$ is the BH amplitude squared. The expressions for $\mathcal{P}_{1,2}(\phi)$ and $\left|\mathcal{A}_{\mathrm{BH}}\left(\xi, t, Q^{2}\right)\right|^{2}$ can be found in 625]. Note that $\left|\mathcal{A}_{\mathrm{BH}}\left(\xi, t, Q^{2}\right)\right|^{2}$ is proportional to the nuclear electric form factor squared $\left(\left|F_{A}(t)\right|^{2}\right)$ and the nucleus charge squared $\left(Z^{2}\right)$.

Integrating the differential cross sections in Eqs. (5.147) and (5.148) over $t$, one obtains the corresponding $t$-integrated cross section $\sigma_{\mathrm{DVCS}(\mathrm{BH})}$ between $t_{\min } \approx-x^{2} m_{N}^{2}$ and $t_{\max }=$ $-1 \mathrm{GeV}^{2}$ :

In fig, 5.61 we present our predictions for a ${ }^{208} \mathrm{~Pb}$ target: in the left plot, the DVCS and BH cross sections at $Q^{2}=4 \mathrm{GeV}^{2}$, in the middle plot the differential cross sections as a function of $|t|$ at fixed $x=5 \times 10^{-3}$, and in the right plot the $A_{L U}$ asymmetry.

In the considered kinematics, the $t$-integrated BH cross section is much larger than the DVCS cross section for $x<10^{-2}$ due to the dramatic enhancement of the BH cross section at small $t \approx t_{\text {min }}$ by the factor $1 / t$, see Eq. (5.148). Therefore, in order to extract a small DVCS signal on the background of the dominant BH contribution for such $x$, one needs to consider the observable differential in $t$. The $t$ dependence of the DVCS and BH differential cross sections has the characteristic shape of the nuclear form factor squared, with distinct minima and maxima. However, the minima of the DVCS cross section are slightly shifted towards smaller $t$ : this is the effect of the leading twist nuclear shadowing in quark nuclear GPDs. The small shift of the minima toward smaller $t$ can be interpreted as an increase of the transverse size of the distributions of quarks in nuclei. One can enhance the effect by using lighter nuclei (e.g., ${ }^{4} \mathrm{He}$ and ${ }^{12} \mathrm{C}$ ) or by considering observables sensitive to the interference between the BH and DVCS amplitudes. For instance, the DVCS beam-spin asymmetry at $A_{\mathrm{LU}}\left(\phi=90^{\circ}\right)$, dramatically oscillates as a function of $|t|$ [994], and the sole reason for these oscillations is the leading twist nuclear shadowing.

Another possibility to study nuclear shadowing in DVCS is offered by processes with nuclear break-up. In this case, the nuclear modification (suppression due to shadowing) of the DVCS break-up cross section (as compared to the impulse approximation) is as large-or even bigger - as that for the coherent case. At the same time, in the impulse approximation,
the relative contribution of the DVCS and BH cross sections is enhanced by $A / Z$ compared to the ep case. It allows one to observe the DVCS signal on the large BH background down to much smaller $x$ than in the ep case, see the discussion in section 3.1.

The leading twist theory of nuclear shadowing allows one also to make predictions for certain observables in exclusive electroproduction of heavy vector mesons $(J / \psi, \Upsilon)$ with nuclear targets which probe the nuclear gluon distribution, with a pattern similar to that discussed for small- $x$ nuclear DVCS 807. See the discussion by M.Strikman in Section 5.8.

### 5.9.2 Nuclear TMDs

Jian-Hua Gao, Zuo-tang Liang, Xin-Nian Wang, Jian Zhou
Transverse momentum dependent distributions (TMDs) were discussed extensively for nucleons earlier in this report. TMDs play an important role in studying final/initial state multiple re-scattering effects in nuclei. Indeed, the leading power nuclear effect comes from the gauge link appearing in the nuclear TMDs, in which the re-scattering effect is encoded.

The extraction of the TMDs from high energy scattering data relies on TMD factorization theorems, established in the $e^{+} e^{-}$annihilation process 241 and semi-inclusive deepinelastic (SIDIS) lepton-nucleon scattering [256]. It is not so clear whether TMD factorization still holds in SIDIS off a large nucleus target. In our recent work [998], we simply assume that it does. Correspondingly, one can introduce leading power unpolarized nuclear TMDs. For simplicity, we restrict our discussion to the light cone gauge, $A^{+}=0$ [263], where

$$
\begin{equation*}
f_{q}^{A}\left(x, \vec{k}_{\perp}\right)=\int \frac{d y^{-}}{2 \pi} \frac{d^{2} y_{\perp}}{(2 \pi)^{2}} e^{i x p^{+} y^{-}-i \vec{k}_{\perp} \cdot \vec{y}_{\perp}}\langle A| \bar{\psi}\left(0, \overrightarrow{0}_{\perp}\right) \frac{\gamma^{+}}{2} \mathcal{L}_{\perp}(0, y) \psi\left(y^{-}, \vec{y}_{\perp}\right)|A\rangle \tag{5.149}
\end{equation*}
$$

and the transverse gauge link is $\mathcal{L}_{\perp} \equiv P \exp \left[-i g \int_{\overrightarrow{0}_{\perp}}^{\vec{y}_{\perp}} d \vec{\xi}_{\perp} \cdot \vec{A}_{\perp}\left(\infty, \vec{\xi}_{\perp}\right)\right]$. This gauge link is not only crucial to ensure the gauge invariance of the TMD parton distribution functions, but also leads to physical consequences such as single-spin asymmetries in SIDIS and the Drell-Yan process in $e+p$ collisions [251, 261, 262]. For DIS off a nucleus target, it should also contain information on the quark transverse momentum broadening due to multiple scattering inside the nucleus 998 .

In the study of either cold or hot nuclear matter, parton transverse momentum broadening plays a crucial role in unraveling the medium properties. One important parameter that controls parton energy loss is the parton transport parameter $\hat{q}$, i.e., the transverse momentum broadening squared per unit of propagation length [999. Therefore, the calculation and measurement of the jet transport parameter is an important step toward understanding the intrinsic properties of the QCD medium. Much effort has been devoted to the study of transverse momentum broadening in high energy collisions within different approaches [999, 1000, 1001, 1002, 1003, 1004, 1005, 1006.

In this contribution, we start from the matrix element definition of the nuclear TMD and identify the gauge link as the main source of leading nuclear effects. The broadened distribution has a Gaussian form, as found in earlier studies [1005], and suppresses the azimuthal asymmetry in SIDIS off nuclear targets. This in turns gives direct experimental access to the cold nuclear matter transport coefficient $\hat{q}$, and offers a way to determine the relative magnitude of the intrinsic transverse momentum in various nucleon TMDs.
Nuclear TMDs and nucleon TMDs. The effect of final state interactions that lead to transverse momentum broadening can be encoded in the gauge link. In fact, the nuclear
dependent part of the quark TMD can be isolated from the gauge link so that the nuclear TMD can be expressed as a convolution of the Gaussian broadening and the nucleon TMD. Assuming a weakly bound nucleon, neglecting the correlation between different nucleons, and keeping only the matrix elements with nuclear enhancement one obtains the nuclear TMD,

$$
\begin{equation*}
f_{q}^{A}\left(x, \vec{k}_{\perp}\right)=\frac{A}{\pi \Delta_{2 F}} \int d^{2} \ell_{\perp} e^{-\left(\vec{k}_{\perp}-\vec{\ell}_{\perp}\right)^{2} / \Delta_{2 F}} f_{q}^{N}\left(x, \vec{\ell}_{\perp}\right), \tag{5.150}
\end{equation*}
$$

as a convolution of the nucleon TMD and a Gaussian with a width $\Delta_{2 F}$ given by the total transverse momentum broadening squared,

$$
\begin{equation*}
\Delta_{2 F}=\frac{1}{A f_{q}^{N}(x)} \int d^{2} k_{\perp} k_{\perp}^{2}\left[f_{q}^{A}\left(x, \vec{k}_{\perp}\right)-f_{q}^{N}\left(x, \vec{k}_{\perp}\right)\right]=\int d \xi_{N}^{-} \hat{q}_{F}\left(\xi_{N}\right) \tag{5.151}
\end{equation*}
$$

where the quark transport parameter $\hat{q}_{F}\left(\xi_{N}\right)$ is defined as

$$
\begin{equation*}
\hat{q}_{F}\left(\xi_{N}\right)=-\frac{g^{2}}{2 N_{c}} \rho_{N}^{A}\left(\xi_{N}\right) \int \frac{d \xi^{-}}{2 p^{+}}\langle N| F_{+\sigma}(0) F_{+}^{\sigma}\left(\xi^{-}\right)|N\rangle=\frac{2 \pi^{2} \alpha_{s}}{N_{c}} \rho_{N}^{A}\left(\xi_{N}\right)\left[x f_{N}^{g}(x)\right]_{x=0}, \tag{5.152}
\end{equation*}
$$

with $\rho_{N}^{A}\left(\xi_{N}\right)$ is the spatial nucleon density inside the nucleus and $f_{g}^{N}(x)$ is the gluon distribution function in a nucleon. Eq. (5.150) is our main result.

Nuclear dependence of azimuthal asymmetry in SIDIS. One can generalize the above approach to the nuclear modification of higher twist TMD parton distributions. The case of twist-3 and twist-4 TMDs [243, 247, 1007, which account for the $\cos \phi$ and $\cos 2 \phi$ azimuthal asymmetries in SIDIS, has been recently investigated in Ref. [1008, 1009]. Here we review the nuclear dependent $\cos \phi$ azimuthal asymmetry in the two kinematic regions: at small transverse momentum $P_{h \perp} \sim \Lambda_{Q C D}$ and intermediate transverse momentum $\Lambda_{Q C D} \ll P_{h \perp} \ll Q$, where $Q$ is the virtual photon momentum. The central ingredient of the treatment in Ref. 1008 is the relation between the nucleon twist-3 TMDs and nuclear ones. If we look at jet production in SIDIS, the azimuthal asymmetry is solely determined by one twist-3 TMD distribution $f^{\perp}\left(x, k_{\perp}\right)$. The ratio of the asymmetry between SIDIS off nucleons and nuclei is,

$$
\begin{equation*}
\frac{\langle\cos \phi\rangle_{e A}}{\langle\cos \phi\rangle_{e N}}=\frac{f_{\perp}^{A}\left(x, k_{\perp}\right) / f^{A}\left(x, k_{\perp}\right)}{f_{\perp}^{N}\left(x, k_{\perp}\right) / f^{N}\left(x, k_{\perp}\right)} \tag{5.153}
\end{equation*}
$$

The ratio depends on how the twist-3 TMD distributions $f_{\perp}^{A}$ is enhanced/suppressed due to the stronger final state interaction taking place inside a nucleus. Following the same approach applied to the twist-2 TMD distribution, we relate the function $f_{\perp}^{A}$ to $f_{\perp}^{N}$,

$$
\begin{equation*}
f_{\perp}^{A}\left(x, k_{\perp}\right) \approx \frac{A}{\pi \Delta_{2 F}} \int d^{2} \ell_{\perp} \frac{\left(\vec{k}_{\perp} \cdot \vec{\ell}_{\perp}\right)}{\vec{k}_{\perp}^{2}} e^{-\left(\vec{k}_{\perp}-\vec{\ell}_{\perp}\right)^{2} / \Delta_{2 F}} f_{\perp}^{N}\left(x, \ell_{\perp}\right) \tag{5.154}
\end{equation*}
$$

Given the TMDs $f^{N}\left(x, k_{\perp}\right)$ and $f_{\perp}^{N}\left(x, k_{\perp}\right)$, one will be able to calculate the ratio (5.154). To illustrate the nuclear dependence of the asymmetry qualitatively, we consider an ansatz of the Gaussian distributions in $k_{\perp}$ for both TMDs,

$$
\begin{equation*}
f^{N}\left(x, k_{\perp}\right)=\frac{1}{\pi \alpha} f_{q}^{N}(x) e^{-k_{\perp}^{2} / \alpha}, \quad f_{\perp}^{N}\left(x, k_{\perp}\right)=\frac{1}{\pi \beta} f_{q \perp}^{N}(x) e^{-k_{\perp}^{2} / \beta} . \tag{5.155}
\end{equation*}
$$

As shown in Fig. 5.62, the azimuthal asymmetry is suppressed in $e+A$ SIDIS as compared to that in $e+N$ SIDIS. Note also that the suppression pattern as a function of $k_{\perp}$ is sensitive to the relative magnitude of the intrinsic transverse momentum in the nucleon TMDs.


Figure 5.62. Ratio $\frac{\langle\cos \phi\rangle_{e A}}{\langle\cos \phi\rangle_{e N}}$ as a function of $\Delta_{2 F}$ for different $k_{\perp}$ and the relative width $\beta / \alpha$.

Now let us discuss the asymmetry at intermediate transverse momentum. The fact that TMDs are perturbatively calculable when $p_{\perp} \gg \Lambda_{Q C D}$ or $k_{\perp} \gg \Lambda_{Q C D}$ allows us to reduce the theoretical uncertainty, since the twist-3 TMDs are poorly known so far. In the parton model, the azimuthal asymmetry for hadron production in SIDIS can be expressed as a convolution of a few TMD distributions and TMD fragmentation functions [243, 247]. It turns out that fragmentation functions $H_{1}^{\perp}$ and $\tilde{H}$ are power suppressed compared to $\tilde{D}_{\perp}$ and $D$ at large $p_{\perp}$ [292, 296, 297]. Therefore, at intermediate transverse momentum, the leading power terms are proportional to $f_{1} \tilde{D}_{\perp}$ and $f_{\perp} D$. In the current fragmentation region, where $p_{\perp}$ is large, we make a collinear expansion around $p_{\perp}=q_{\perp}$ in terms of the power $k_{\perp} / q_{\perp}$ and keep the quadratic terms $k_{\perp}^{2} / q_{\perp}^{2}$ in order to extract the nuclear dependent contributions. After carrying out the integrals over $p_{\perp}$, we find the nuclear dependent azimuthal asymmetry is related to the term $D(z) \int \frac{k_{\perp}^{2}}{q_{\perp}^{2}} f_{1}\left(x, k_{\perp}\right) d^{2} k_{\perp}$. Therefore, the difference of the $\cos \phi_{h}$ azimuthal asymmetry is proportional to the transverse momentum broadening.

$$
\begin{equation*}
\left\langle\cos \phi_{h}\right\rangle_{e A}-\left\langle\cos \phi_{h}\right\rangle_{e N} \propto \int \frac{k_{\perp}^{2}}{q_{\perp}^{2}}\left[f_{1}^{A}\left(x, k_{\perp}\right)-f_{1}^{N}\left(x, k_{\perp}\right)\right]=\frac{\Delta_{2 F}}{q_{\perp}^{2}} \tag{5.156}
\end{equation*}
$$

Conclusions. In summary, we can get a direct handle on the crucial transport parameter $\hat{q}$, which descrcibed the properties of the QCD medium, by measuring the nuclear dependent azimuthal asymmetry at intermediate transverse momentum. Conversely, the target nucleus can be used as a filter to study nucleon TMDs, e.g., to determine the relative magnitude of the intrinsic transverse momentum of $f^{N}$ and $f_{\perp}^{N}$.

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### 5.10 Current fragmentation

## Introduction and the role of $e+A$ collisions

Raphaël Dupré and Alberto Accardi
The fragmentation process, by which hard partons turn into hadrons, is only partly known due to its non perturbative nature. Fragmentation functions, which encode the probability that a parton fragments into a hadron, have been obtained by fitting experimental data covering large kinematic ranges and numerous hadron species, see Section 5.10. However, knowledge about the dynamics of hadronization remains fragmentary: this process has been studied in a number of model calculations, but lacks a first-principles description in QCD. One possible scenario for the hadronization process is sketched in figure 5.63 as an example for DIS. At LO the virtual photon strikes a quark, which then propagates quasifreely emitting gluons; after a time called production time, the quark neutralizes its color and gluon emission stops. The quark becomes a pre-hadron, which will eventually form a hadron at the formation time. In fact, a color string connects the struck quark to its nucleon, and hadrons can be formed all along this string, but we focus our attention on the hadron that contains the struck parton. In nuclear DIS, the hadronization process happens at least in part in the target nucleus (cold nuclear matter). Thus the quark is subject to energy loss by medium-induced gluon brehmsstrahlung, and the prehadron (as well as the hadron) can have inelastic interactions with the surrounding nucleons, leading to attenuation and broadening of the produced particle spectra. The relative weight of one mechanism compared to the other is determined by the magnitude of the color neutralization time. For full reviews, see Refs. [1010, 1011, 1012]. Alternative scenarios are also feasible and final states in nuclear DIS (nDIS) can help untangle these from the scenario outlined here to provide genuine insight into the hadronization process.


Figure 5.63. A model sketch of the hadronization process.
These nuclear effects are both an opportunity for a first principles study hadronization and nuclear properties as well as important benchmarks for reducing existing uncertainties in many nuclear measurements. For example, in neutrino experiments, nuclei are used to maximize the cross section and the kinematics are reconstructed from the hadronic final state. Therefore, a poor knowledge of hadron attenuation leads to a tangible systematic error. In heavy-ion collisions, hadrons are produced in hot and expanding nuclear matter, whose properties can be measured, among other methods, by the modifications of highenergy particle spectra compared to proton-proton and proton-nucleus collisions. It is clear that the details and the time scales of the hadronization process can profoundly modify the interpration of the data, see Fig. 5.2,

The role of $e+A$ collisions. Nuclear deep inelatic scattering provides a known and stable
cold nuclear medium and a low-multiplicity final state with strong experimental control on the kinematics of the hard scattering. This permits one to use nuclei as femtometer-scale detectors and study the time scales of the hadronization process and calibrate theoretical models for parton energy loss and prehadronic scattering, that can then be applied, for instance, to the study of the QGP, see Figure 5.2, Initial state parton energy loss can furthermore be studied in isolation from hadronization in Drell-Yan lepton pair production in $p+A$ collisions, where however it can be masked by nuclear modification of the target wave function such as antishadowing and the EMC effect. So, an interplay of nuclear DIS and nuclear Drell-Yan can help isolate hadronization effects on one hand, and on the other to clarify the differences in quark and anti-quark antishadowing. Perhaps more interestingly, the study of hadronization in nuclear DIS can give direct information about the gluon structure of the nuclei. For example, one can link energy loss and transverse momentum broadening to the gluon density [1013] or more directly to the saturation scale [801]. In models like GiBUU [1014, focussing on hadron absorption, access to the pre-hadron evolution and its color transparency evolution is possible. All these physical interpretation of the data are model dependent and based on very different assumptions about the relative importance of the interaction mechanisms, therefore they are fragile and need to be carefully validated and calibrated with precise data.

The typical observables used to explore hadronization in nuclear DIS are the multiplicity ratio and the transverse momentum broadening, in both cases they are comparison of deuterium with heavier nuclei. The multiplicity ratio, representing the production rate of a hadron $h$ in a nuclear target $A$ compared to Deuterium, is defined as

$$
\begin{equation*}
R_{A}^{h}\left(Q^{2}, \nu, z_{h}, p_{T}^{2}\right)=\frac{N_{A}^{h}\left(Q^{2}, \nu, z_{h}, p_{T}^{2}\right) / N_{A}^{e}\left(Q^{2}, \nu\right)}{N_{D}^{h}\left(Q^{2}, \nu, z_{h}, p_{T}^{2}\right) / N_{D}^{e}\left(Q^{2}, \nu\right)} \tag{5.157}
\end{equation*}
$$

with $N_{t}^{e}$ and $N_{t}^{h}$ respectively the number of electrons and the number of semi-inclusive hadrons $h .1-R_{A}^{h}$ is the attenuation of hadron production in a nucleus of atomic mass $A$. This ratio minimizes the influence of nuclear PDF modifications, which have been shown to cancel to a large degree up to NLO. The hadron transverse momentum broadening, representing the increase of transverse momentum in a nuclear target A compared to Deuterium, is defined by $\Delta\left\langle p_{T}^{2}\right\rangle=\left\langle p_{T}^{2}\right\rangle_{A}-\left\langle p_{T}^{2}\right\rangle_{D}$, with $\left\langle p_{T}^{2}\right\rangle_{t}$ the average hadron transverse momentum measured in a nucleus. When integrated over a large kinematic range, these observables they are dominated by the geometry of the nuclei and do not discriminate well between the models. One needs to also consider more differential observables, including a multi-dimensional analysis of $R_{M}$ and $\Delta\left\langle p_{T}^{2}\right\rangle$, and hadron-hadron and photon-hadron correlations.

Another possibility is to use experimental settings in which we can isolate the involved processes. In the case of EIC, the high energy boost imparted to the struck quark in events with large $\nu$ can increase dramatically the production length, which leads to prehadron production far outside the nuclei and an experimental isolation of pure parton energy loss effects. Since the pre-hadron production time is expected to roughly be inversely proportional to the mass squared of the hadron, measuring attenuation and $p_{T}$-broadening of many meson and baryon species, together with the large $\nu$ leverage afforded by the EIC, will give another important handle in the exploration of the hadronization mechanism. New features will be availabe at the EIC, the high rate for heavy flavor production ( $D$ and $B$ mesons) will allow the measurement of heavy quark energy loss. Finally, jet production, will open the possibility to study the dynamics of parton showers and the detailed transport properties of cold nuclear matter using specific jet observables.

Overview of theoretical models. Three processes are typically included in theoretical descriptions of in-medium hadronization: quark energy loss, pre-hadron absorption and modified fragmentation functions. The models in the literature are usually based on one or two of those and neglect the others. In this section we will discuss a few examples to give an idea of the abundant existing literature; for a detailed review, including models specific to heavy-ion collision experiments, see Ref. [1010].

Pure quark energy loss models assume a very long production time and are typically used to describe hadron suppression in the hot nuclear matter produced in heavy-ion collision. In a few cases they have been applied to nDIS data as well [1015, 1016 permitting a common interpretation of hadron suppression in cold and hot nuclear matter. In these models, hadron suppression is due to the lower energy of the quark when it fragments, so that hadrons are produced in lower number and at lower energy. The differences in the models depend on the way calculations of medium-induced gluon radiation are performed, on the modeling of the medium, and on assumptions about its coupling to the hard parton.

Typically, parton energy loss is determined by the transport coefficient $\hat{q}$, which is defined as the transverse momentum square transfered to a quark after propagating through a length of nuclear matter and is a characteristic property of that matter. It is expected to be much larger in a Quark-Gluon Plasma than in the nucleus of a nDIS experiment, which is what is observed from the analysis of experimental data from RHIC and HERMES [1015, 1016, 1017, 1018. The $\hat{q}$ transport coefficient is directly related to the observed broadening of the $p_{T}$ distribution of hadrons in nDIS; it follows that the main challenge for these pure energy loss models is to make a coherent picture of both multiplicity ratios and hadron $p_{T}$ broadening. In particular, for some of the models, the $\hat{q}$ extracted from multiplicity ratios is larger by an order of magnitude than what one would estimate from the hadron transverse momentum broadening. This has led some authors 1019 to the conclusion that quark energy loss is not enough to explain the observed nuclear effects; nevertheless, the variation between theoretical models is still too big for a definitive statement.

The GiBUU model [1014] is an absorption model based on Boltzmann equation including only hadronic and pre-hadronic interactions, see Section 5.10. It assumes short productions times obtained from the Lund string model and neglects gluon brehmstralung from the partonic stage. It can describe very well well most of the hadron multiplicity ratios measured at HERMES and EMC using a linear growth of the pre-hadron cross section between production time and formation time. Other pure absorption models [1020, 1021, 1022] are also successful in describing hadron attenuation. However, the transverse momentum broadening remains a challenge for this kind of models; some progress within GiBUU has been presented during the meeting by Kai Gallmeister.

To resolve the problems of the previous "pure" models, Kopeliovich et al. [1019] describe hadronization including both quark energy loss and hadron absorption. In their model, the transverse momentum broadening is linked to quark energy loss and the multiplicity ratio suppression is explained by hadron absorption, therefore the two processes can be independently quantified. This model describes HERMES data to a large extent, and highlights the fact several processes are involved and need to be disentangled.

Recently, HERMES data have also been described by assuming factorization and universality to hold at the nuclear level not only for parton distributions but also for fragmentation functions, and a set of nuclear Fragmentation Functions have been fitted to experimental data using both $e+A$ interactions and $d+A u$ collisions at RHIC. In this case, no dynamical assumption is made of the physical mechanism for nuclear modifications of hadron production; this information is subsumed into the non-perturbative nuclear FFs-see Section


Figure 5.64. Multiplicity ratio of positively charged hadrons (left) and negatively charged hadrons (right) from the HERMES experiment [1029]
5.10

A number of other models exist using different variants of the discussed mechanisms, and most of them are able to describe the existing data to a good extent: no consensus is reached yet on which mechanisms are dominant, and indeed this is the main motivation for future precise measurements of hadronization at Jefferson Lab [1023], which will be completed by the time EIC starts its operations, and will help settle some of the issues related to early time color dynamics and interaction in cold nuclear matter.
Previous mesurements and open questions. Unidentified charged hadron multiplicity ratios in nuclei were measured in numerous lepton facilities, the earlier results were by Osborne et al. [1024] at SLAC, Hand et al. 1025] and the E665 collaboration [1026] at FNAL, and the European Muon Collaboration [1027, 1028 at CERN. Those measurements revealed a general picture: hadron suppression is stronger at low $\nu$ and high $z$. On the opposite side, at low $z$, an increase of the number of hadron is observed.

In the more recent data from the HERMES collaboration [1029, 1030] several hadrons are studied individually (Fig. 5.64), and new observables such as transverse momentum broadening (figures 5.67 and 5.68) and two hadrons multiplicity ratios 1031 are measured. Because of their improved precision and the large number of hadron species, these data provide us today with a much more detailed picture, which leads to new questions. The behavior of the kaons, for example, is very interesting: $\mathrm{K}^{+}$are less suppressed than pions, but $\mathrm{K}^{-}$have the same behavior as pions (figure 5.64). This difference is not reproduced by existing models, showing that the relatively simple phenomenological models utilized so far cannot fully describe the data. Furthermore, the introduction by HERMES of precise and flavor dependent $\Delta p_{T}^{2}$ measurement [1030] has revealed another strange behavior: the $p_{T}$ broadening of $K^{+}$is larger than for the pion (Figure 5.67 right). This seems to indicate more interaction for kaons, and yet they are less suppressed. To solve this apparent incongruity, one may have to consider models based on different processes involved at different
stages of hadronization, like in Reference [1019], reinforcing the indications coming from kaon suppression. Furthemore, no model is able to describe the $z$ dependence of the $p_{T}$ broadening, highlighting once again the need for a more detailed theoretical understanding of hadronization. Finally, proton observables are very different from anti-protons (figure 5.64), and no model is yet able to reproduce them correctly, although few attempts have been made [1014, 1032]. At the low energies of HERMES, part of the problem may be due to protons coming from the target fragmentation region, which is interesting in its own right. The collider geometry and the large energy range of EIC will permit to experimentally separate clearly target and current fragmentation, allowing to address hadronization in either region. Indeed developing a consistent picture within a given model for both current and target fragmentation would be a great theoretical progress.

To complete the review of existing data, we should mention the preliminary results on pion and kaon production from the CLAS collaboration at Jefferson Lab, where electrons up to 5 GeV scatter on fixed targets ranging from Carbon to Lead [1033, 1034].

## Studying hadronization at an EIC

## Raphaël Dupré and Alberto Accardi

The experimental study of the hadronization process using nDIS is well established; however the high energy available at the EIC creates novel opportunities. The main interest in going at higher energy is to ensure that hadron formation occurs outside of the nuclei, in order to isolate in-medium parton interactions and energy loss. Furthemore, an EIC will permit, for the first time in $e+A$ collisions, the study of hadronization of the open charm and eventually open bottom mesons. Recent results from RHIC [1035, 1036] are showing unexpected results for open charm and bottom suppression in $A+A$ collisions, and several contrasting explainations have already been suggested, with more detailed experiments planned at RHIC. However, due to the intricated interplay of the many variables in $A+A$ collisions and to the poorly known nature of the Quark-Gluon Plasma partons, the $e+A$ input seems necessary to confirm any interpretation. Also, the considerable energy leverage offered by an EIC is a chance to map precisely the $Q^{2}$ evolution of parton energy loss, and determine possible nuclear modifications of DGLAP evolution. The high luminosity will also facilitate the study of two particle correlations (such as hadron-hadron or photon-hadron) over a wide energy range, largely improving recent HERMES measurements, and complementing the low-energy measurements planned at CLAS. Finally, high energy permits access to jets, which give an opportunity to use new observables with improved sensitivity to quark energy loss and the medium modification of fragmentation functions, see Section 5.11. They also facilitate a detailed determination of the cold nuclear matter transport coefficients, which encode basic information on the non perturbative gluonic structure of the nuclei and can be calculated from first principles, e.g., in lattice QCD [1037].

To illustrate the possibilities offered by EIC, we show projections done using the PYTHIA Monte-Carlo generator to evaluate cross sections at $s=200$ or $1000 \mathrm{GeV}^{2}$, and $L=$ $200 \mathrm{fb}^{-1}$. We apply a series of cuts on the generated events to ensure the DIS nature of the interaction $\left(Q^{2}>1 \mathrm{GeV}^{2}\right.$ and $\left.W^{2}>4 \mathrm{GeV}^{2}\right)$, to limit radiative corrections ( $y<0.85$ ), to insure that we can detect the scattered electron $(y>0.1)$ and to limit di-parton production in the hard scattering of the virtual photon $\left(x_{B j}>0.1\right)$. Finally we assume an acceptance of $50 \%$ for pions, eta meson and kaons, and, an acceptance of $2 \%$ for heavy mesons. The acceptance is set low for heavy mesons to account for the small number of decay channels


Figure 5.65. Multiplicity ratio in function of z for various $\nu$ bins. Full points are data from HERMES [1029, empty are projections for statistical errors at the EIC, at arbitrary vertical position. The left panel shows EIC measurements at $s=200 \mathrm{GeV}^{2}$, for 2 different $\nu$ cuts $(20<\nu<30 \mathrm{GeV}$ and $50<\nu<70 \mathrm{GeV}$ ); the right panel at $s=1000 \mathrm{GeV}^{2}$ with $100<\nu<130 \mathrm{GeV}$.
that can be effectively detected. EIC observables are plotted on arbitrary vertical scales, and include statistical errors only.

An EIC is the perfect tool for precise measurement of quark energy loss and transverse momentum broadening. One may object that at the higher EIC energies, because of the large $\nu \gtrsim 150 \mathrm{GeV}$, the relative effect on the quark momentum is too little to produce an appreciable hadron attenuation. This is true at least for the pions, as shown by EMC data. However, attenuation may in fact disappear at a yet higher value of $\nu$ for large $z$ or for heavier particles, because of reduced production times, or for large $Q^{2}$, because of a faster evolution in virtuality as discussed in Section 5.11. Anyway, because of the EIC kinematic flexibility, interesting multiplicity ratios can be measured. For example, Figure 5.65 shows projections for light and heavy flavors, which would shed light on the heavy quarks at RHIC, where they unexpectedly display a similar suppression compared to their light counterparts. It is also interesting to compare mesons of different mass but the same valence quark contents, such as $\pi^{0}$ vs. $\eta$, and $K^{0}$ vs $\Phi$. Figure 5.66 shows projections for the former case compared to calculations in a pure energy loss or pure prehadron absorption scenario. The sensitivity of such measurement to the hadronization time scales is obvious.

Changing observables, measurements of the hadron transverse momentum broadening permit getting around the small values of hadron attenuation at large energies. Indeed the $p_{T}$ broadening to first approximation is independent of $\nu$, and even very little effects can be experimentally observed; moreover, the induced transverse momentum has a theoretical interpretation in terms of transport coefficients. However, one should keep in mind that $\Delta\left\langle p_{T}^{2}\right\rangle$ of pions or other hadrons is not a direct measurement of $\hat{q}$, which is the parton transverse momentum broadening, and that it is essential to use dependences in $\nu$ and $z$ to make a model independent extraction of $\hat{q}$. One may also access $\hat{q}$ through nuclear modifications of hadron azimuthal asymmetries, see Section 5.9.2. The importance of this topic, especially in the scope of other EIC measurements, is enhanced by the connection between $\hat{q}$ and the saturation scale 801, enabling an independent large- $x$ measurement of the latter, complementary to the more traditional small- $x$ measurements discussed in Section 5.2, An EIC will not only allow one to make those measurements with pions but


Figure 5.66. Multiplicity ratio for $\pi^{0}$ and $\eta$ mesons compared to pure energy loss and pure prehadron absorption computations.


Figure 5.67. Transverse momentum broadening in function of z (left) and A (right), empty triangles and star are projections for EIC at $s=1000 \mathrm{GeV}^{2}$, full points are HERMES data.
also, and uniquely compared to previous $\mathrm{e}+\mathrm{A}$ facilities, with heavy mesons (see figures 5.67).

The $Q^{2}$ evolution of hadron attenuation is not clearly understood: HERMES data indicate a small rise of the transverse momentum broadening, but the $Q^{2}$ coverage is not large enough to make a definite statement. An EIC can do a far better job as shown in figure 5.68 and provide a unique probe to detect any modification of the DGLAP evolution in nuclear medium.

The scaling of the hadronization times and the quark energy loss with the mass of quarks is an important question that can be used to reveal pQCD effects in parton energy loss and non perturbative effects in hadronization [1038, 1039. Many measurements to explore this at the EIC are possible, as the figures in this section illustrate.

To achieve the discussed measurement the key experimental requirement are good particle ID in general; for heavy flavors one needs in particular a very good vertex detector resolution, which needs to be of the order of few tens of micrometer, and high luminosity to reach a statistical precision allowing unambigous theoretical interpretations. Having a $\nu$ range covering low values for studies of hadronization and large values for studies of parton propagation and energy loss will require energies spanning $s=200-1000 \mathrm{GeV}^{2}$. The


Figure 5.68. Multiplicity ratio (left) and transverse momentum broadening (right) in function of $Q^{2}$, empty markers are projections for EIC at $s=200 \mathrm{GeV}^{2}$ (triangles) and at $s=1000 \mathrm{GeV}^{2}$ (circles), full markers are HERMES data.
lowest required energy can be increased provided measurements of $y<0.1$ can be achieved for SIDIS observables.

Finally, the high energy of an EIC provides the chance, for the first time in $e+A$ collisions, to study hadronization through jet observables. Jets are a new and independent way to access transport coefficient $\hat{q}$ and confirm other measurements, to explore in detail the medium induced gluon radiation and transport properties of cold nuclear matter, and to study the conversion of the parton shower into hadrons, see Section 5.11.

## Hadronization in $e+A$ collisions within GiBUU

## Kai Gallmeister and Ulrich Mosel

The study of the interaction of hadrons, produced by elementary probes in a nucleus, with the surrounding nuclear medium can help to investigate important topics, such as color transparency and hadronization time scales. We investigate this by means of the semiclassical GiBUU transport code 1040, which not only allows for the absorption of newly formed hadrons, but also for elastic and inelastic scattering as well as for side feeding through coupled channel effects. A study of parton interactions in cold, ordinary nuclear matter of known properties is important to disentangle effects of the interaction of partons from those of the medium in which they move.

We summarize here the main features of our model, for details see [1014]. The model relies on a factorization of hadron production into the primary interaction process of the lepton with a nucleon, essentially taken to be the free one, followed by an interaction of the produced hadrons with nucleons. We have modeled the prehadronic interactions such that the description is applicable at all energy regimes and describes the transition from high to low energies correctly. For the first step, we use the PYTHIA model that has been proven to very successfully describe hadron production, also at the low values of $Q^{2}$ and $\nu$ treated in our studies. This model contains not only string fragmentation but also direct interaction processes such as diffraction and vector-meson dominance. In this first step, we take nuclear effects such as Fermi motion, Pauli blocking and nuclear shadowing into account [1041. The relevant production and formation times 1014 are obtained directly from PYTHIA [1042. In the second step we introduce prehadronic interactions between


Figure 5.69. Nuclear modification factor for charged hadrons. Experimental data are shown for HERMES at 27 GeV and for EMC at $100-280 \mathrm{GeV}$. The cross section scenarios are (from left to right): constant, linear and quadratic increase with time after production.
the production and the formation time and the full hadronic interactions after the hadron has been formed.

The actual time dependence of the prehadronic interactions presents an interesting problem in QCD. Dokshitzer et al. 1043 have pointed out that QCD and quantum mechanics lead to a time-dependence somewhere between linear and quadratic. We also note that a linear behavior has been used by Farrar et al. [1044] in their study of quasi-exclusive processes. In our calculations, we work with different time-dependence scenarios, among them a constant, lowered pre-hadronic cross section, a linearly rising one, and a quadratically rising one. In addition, we study a variant of the latter two, where the cross section for leading hadrons, i.e., hadrons that contain quarks of the original target nucleon, starts from a pedestal value $\sim 1 / Q^{2}$, thus taking into account possible effects of color transparency.

Fig. 5.69 shows a comparison of these various model assumptions to HERMES and EMC data on unidentified charged hadron attenuation. A good description of both data sets simultanousely is obtained only with a linear time dependence of the cross sections. Furthermore, a nearly perfect agreement is observed in HERMES data for pions, kaons, and protons, which


Figure 5.70. The average formation time of different particles divided by $\nu$ as a function of $\nu$ for several experimental setups. give the attenuation $R_{M}$ as a function of energy transfer $\nu$, relative energy $z_{h}=E_{h} / \nu$, momentum transfer $Q^{2}$ and the squared transverse momentum $p_{T}^{2}$ [1029. The rise of $R_{M}$ with $\nu$ is mainly an acceptance effect, as we have shown in [1041], whereas the weaker rise of $R_{M}$ with $Q^{2}$ reflects the pedestal value $\sim 1 / Q^{2}$ of the pre-hadronic cross sections.

In Fig. 5.70 we show the average formation time for different particle species as a function of the boson energy $\nu$. One realizes a smooth transition from CLAS at 5 GeV up to EMC at 280 GeV for all particle species. One observes a somehow larger formation time for pions than for the heavier particles. Nevertheless, this effect, being somewhere on a $50 \%$
level, is much smaller than mass ratios would suggest: $m_{N} / m_{\pi} \sim 7$. Thus, recalling the basic boost relation, $t_{h}=\gamma_{h} \tau_{h}=\left(E_{h} / m_{h}\right) \tau_{h}$, the factor $\tau_{h}$ and the factor $m_{h}$ in the nominator/denominator cancel each other. We therefore conclude that, within our model, the formation time of a hadron in its rest frame is proportional to its mass, $\tau_{f} \propto m_{H}$, contrary to common assumptions of a constant formation time for all hadron species, which can also be obtained from uncertainty principle considerations [1038, 1010].


Figure 5.71. The hadron attenuation for different hadron species within several $Q^{2}$ bins as function of $z$ (left panel) and $\nu$ (for $z>0.2$, right panel) for a collider setup $(3+30) \mathrm{GeV}$.

Hadron Attenuation at an EIC: Strong $Q^{2}$ Dependence. One may now look at hadron attenuation at an EIC. Fig. 5.71shows the expected attenuation for different hadron species within several $Q^{2}$ bins as functions of $\nu$ and $z$ for a very low energy collider setup $(3+30) \mathrm{GeV}$, which is close to former EMC conditions. One observes a large $Q^{2}$ dependence: while for low $Q^{2}$ values, the attenuation of all hadron species decreases to approx. 0.5 at $z \rightarrow 1$, the attenuation is only approx. 0.8 for $Q^{2}>4 \mathrm{GeV}^{2}$. This is also shown in Fig. 5.71, where the same attenuation is shown, but now as a function of $Q^{2}$ and integrated over all $\nu$ and $z>0.2$ values. It is worthwhile mentioning that there is nearly no $\nu$ dependence for all $Q^{2}$ bins visible in our calculations.
Hadron Attenuation at an EIC: $\boldsymbol{\pi}^{0}$ vs. $\boldsymbol{\eta}$. As already shown in Fig. 5.71, some differences in the resulting attenuation ratio show up for different hadron species. In Section 5.10, it has been suggested that a comparison of $\eta$ and $\pi^{0}$ attenuation ratios will distinguish between energy-loss models and absorption models. In Fig. 5.72 we show our results for the attenuation of these two particle species. Both attenuation signals are close to each other, but show stronger absorption for $\pi^{0}$ than for $\eta$ mesons, in which case the discriminatory power would weaken. In Fig. 5.72 we also show the hadronic interaction cross section of pions and eta mesons with nucleons. For laboratory momenta larger than 2 GeV , these are nearly identical. Thus differences in the attenuation are due to formation time effects.

## A global fit of nuclear fragmentation functions

## Rodolfo Sassot, Marco Stratmann, Pia Zurita

Similarly to modifications of PDFs in nuclei, the production of hadrons in the finalstate is known to be affected when occurring in a nuclear environment. For example,


Figure 5.72. Left panel: The hadron attenuation for $\pi^{0}$ and $\eta$ mesons for a collider setup of $3+30$ GeV. Right panel: The hadronic interaction cross section of $\pi^{0}$ and $\eta$ mesons with nucleons at rest as a function of the meson momentum.
semi-inclusive deep-inelastic scattering (SIDIS) off large nuclear targets shows significant differences as compared to hadron production off light nuclei or proton targets, as reviewd in Section 5.10.

The past few years have seen a significant improvement in the pQCD description of hadron production processes, and, more specifically, in the precise determination of vacuum fragmentation functions (FFs), including estimates of their uncertainties [74. FFs carry the details of the non-perturbative hadronization process, factorized from the hard scattering cross section in the same way as for PDFs. The most important result of these studies is that the standard pQCD framework not only reproduces data on electron-positron annihilation into hadrons, but it describes with remarkable precision also other processes like semiinclusive deep-inelastic scattering and hadron production in proton-proton collisions. It is then quite natural to ask if pQCD factorization can be also generalized to final-state nuclear effects, i.e., to introduce medium modified or nuclear fragmentation functions ( nFFs ), and to assess how good such an approximation works or to determine where and why it breaks down. From theoretical considerations alone, the answer is, however, not obvious since on the one hand, interactions with the nuclear medium may spoil the requirements of the factorization theorems, but, on the other hand, any estimates of possible factorization breaking effects are strongly model dependent.

Within the factorization ansatz, nFFs should contain (factorize) all the non-perturbative details related to hadronization in a nuclear environment, would be exchangeable from one process to another (universal), and would allow for QCD estimates at any given order in perturbation theory in a well defined and unified framework. These features can be explicitly tested using data from an increasing but still limited number of experiments that have performed precise measurements of hadron production off nuclear targets, for instance, in SIDIS by HERMES [1029] or in deuteron-gold collisions studied at RHIC [1045, 1046]. Both type of processes are compatible with a universal nuclear modification of the hadronization mechanism in the currently accessible kinematic regime. The inclusion of next-to-leading order QCD corrections and the possibility to use different observables have been proven to be crucial for an accurate parametrization of nFFs 967.

In addition to the primary goal of testing the factorization properties of nFFs and to constrain them from different data sets in a consistent theoretical framework (for further comparison with the different model estimates), a thorough analysis of nFFs also serves as a baseline for ongoing studies of hadron production processes in heavy-ion collisions performed at RHIC and the LHC [1047. In the following, we present a brief summary


Figure 5.73. Quality of the nFF fit to nuclear SIDIS data from HERMES.
of the first global fit of nFFs and outline limitations in the analysis imposed by the data available so far.
Medium Modified Fragmentation Functions. Even though nuclear effects in the hadronization process have been known to be significant for quite some time, only recent experiments have become precise enough and selective from a kinematical point of view to allow for more detailed and quantitative studies. Specifically, the HERMES collaboration has performed a series of measurements of pion, kaon and proton attenuation on different nuclear targets as a function of the hadron momentum fraction $z$ and the photon virtuality $Q^{2}$, which both are used to characterize fragmentation functions, as well as the virtual photon energy $\nu$, that can be related to the nucleon momentum fraction $x$ carried by initial-state parton, see Fig. 5.64,

Single-inclusive identified hadron yields obtained in $d+A u$ collisions at mid-rapidity at BNL-RHIC, which show a characteristic nuclear suppression and enhancement pattern as a function of the hadron transverse momentum $p_{T}$, are another source of information on nuclear modification effects in the hadronization process. These measurements are often


Figure 5.74. Comparison of medium modified and standard FFs.
seen as "control experiments" associated with the heavy-ion program at RHIC to explore the properties of nuclear matter under extreme conditions. However, in view of the evidence for strong medium induced effects in the fragmentation process found in SIDIS, $d+A u$ data are also of particular relevance for extracting nFFs and testing the assumed factorization and universality properties.

To perform global nFF fits, it was proposed in Ref. [967] to relate the medium modified fragmentations to the standard ones in a convolution approach with a very simple ansatz for the weight functions. The fits gives a very good description of the full kinematic dependence of the HERMES data as can be seen in Fig. 5.73 while an approach which ignores all finalstate nuclear effects clearly fails. The same set of nFFs that account for nuclear modification in SIDIS also reproduce the main features of the $d+A u$ data from RHIC. The peculiar $p_{T}$ dependence of the effects is found to come from an interplay between quark and gluon fragmentation as a function of $p_{T}$ in the hadron production cross section. It is interesting to notice that there seems to be no visible conflict between the standard $Q^{2}$ dependence assumed for the nFFs and the data. In this respect, there have been many interesting suggestions and model dependent calculations at the LO level, motivating the use of medium modified evolution equations. However, in the range of $Q^{2}$ covered by present SIDIS and $d+A u$ data, there is no evidence for any significant departure from standard time-like evolution equations [1048, 1049, 1050, 1051].

The pattern of medium induced modifications is rather different for quarks and for gluons, see Fig. 5.74. The dominant role of quark fragmentation in SIDIS leads to a suppression, i.e., $R_{q}^{\pi}<1$, increasing with nuclear size $A$ as dictated by the pattern of hadron attenuation found experimentally. The enhancement of hadrons observed in $d+A u$ collisions for $p_{T} \approx 10 \mathrm{GeV}$, along with the dominant role of gluon fragmentation at low values of $p_{T}$ explains that $R_{g}^{\pi}>1$ for $z \rightarrow 0.2$. Below $z \simeq 0.2$, where all the data used in the fit have very limited or no constraining power, both quark and gluon nFFs drop rapidly. For the time being, the behavior in this region could easily be an artifact of the currently assumed functional form for the parameterization. The extended $Q^{2}$ range of EIC will allow one to accurately test the factorization assumption for nFFs , which is at the basis of the presented approach to nuclear modfications of hadron production.

## Heavy quarks and quarkonia in a nuclear environment

## B. Z. Kopeliovich

Time dependence of vacuum radiation. The color field of a quark originating from a hard reaction (DIS, high- $p_{T}, e^{+} e^{-}$, etc.) is stripped off, i.e., such a quark is lacking a color field up to transverse frequencies $q \lesssim Q$, and starts regenerating its field by radiating gluons, i.e., forming a jet. This can be described by means of an expansion of the initial "bare" quark over the Fock states containing a physical quark and different number of physical gluons with different momenta. Originally, this is a coherent wave packet equivalent to a single bare quark $|q\rangle$. However, different components have different invariant masses and they start gaining relative phase shifts as a function of time. As a result, the wave packet is losing coherence and gluons are radiated in accordance with their coherence times. The required time is to the jet energy, since the radiation time (or length) depends on the gluon energy and transverse momentum $k$ (relative to the jet axis),

$$
\begin{equation*}
l_{c}=\frac{2 E}{M_{q g}^{2}-m_{q}^{2}}=\frac{2 E x(1-x)}{k^{2}+x^{2} m_{q}^{2}} . \tag{5.158}
\end{equation*}
$$

Here, $x$ is the fractional light-cone momentum of the radiated gluon; $m_{q}$ is the quark mass; $M_{q g}^{2}=m_{q}^{2} /(1-x)+k^{2} / x(1-x)$ is the invariant mass squared of the quark and radiated gluon.

One can trace how much energy is radiated over the path length $L$ by the gluons which have lost coherence during this time interval [1052, 1019, 1053, 1054, 1055,

$$
\begin{equation*}
\Delta E(L)=E \int_{\Lambda^{2}}^{Q^{2}} d k^{2} \int_{0}^{1} d x x \frac{d n_{g}}{d x d k^{2}} \Theta\left(L-l_{c}\right) \tag{5.159}
\end{equation*}
$$

where $Q \sim p_{T}$ is the initial quark virtuality; the infra-red cutoff is fixed at $\Lambda=0.2 \mathrm{GeV}$. The radiation spectrum reads

$$
\begin{equation*}
\frac{d n_{g}}{d x d k^{2}}=\frac{2 \alpha_{s}\left(k^{2}\right)}{3 \pi x} \frac{k^{2}\left[1+(1-x)^{2}\right]}{\left[k^{2}+x^{2} m_{q}^{2}\right]^{2}} \tag{5.160}
\end{equation*}
$$

where $\alpha_{s}\left(k^{2}\right)$ is the running QCD coupling, which is regularized at low scale by the substitution: $k^{2} \Rightarrow k^{2}+k_{0}^{2}$ with $k_{0}^{2}=0.5 \mathrm{GeV}^{2}$. In the case of heavy quark the $k$-distribution Eq. (5.160) peaks at $k^{2} \approx x^{2} m_{q}^{2}$, corresponding to the polar angle (in the small angle approximation) $\theta=k / x E=m_{q} / E$. This is known as the dead cone effect [1056, 1057].

The step function in Eq. (5.159) creates another dead cone [1055): since the quark is lacking a gluon field, no gluon can be radiated unless its transverse momentum is sufficiently high, $k^{2}>2 E x(1-x) / L-x^{2} m_{q}^{2}$. This bound relaxes with the rise of $L$ until it reaches $k^{2} \sim x^{2} m_{q}^{2}$, characterizing the heavy quark dead cone at $L_{q}=E(1-x) / x m_{q}^{2}$. The radiation of such a "naked" quark has its own dead cone controlled by its virtuality $Q^{2} \gg m_{q}^{2}$, and is much wider than the one related to the quark mass. Therefore, there is no mass dependence of the radiation until the quark virtuality cools down to $Q^{2} \Rightarrow Q^{2}(L) \sim m_{q}^{2}$. At the early stage of hadronization, when $Q^{2}(L) \gg m_{q}^{2}$, all quarks radiate equally, and the results of [1057] for a reduced energy loss of heavy quarks should be applied with a precaution. The numerical results demonstrating this behavior are depicted in Fig. 5.75,

One can see that a substantial difference between the radiation of energy by charm and light quarks onsets at rather large distances, above 10 fm . However the $b$-quark radiation is suppressed already at a short distance, less than one fermi. Moreover, it completely regenerates the color field already at a distance of the order of 1 fm



Figure 5.75. Left panel: Vacuum energy loss by light $\left(m_{q}=0\right)$, charm ( $m_{c}=1.5 \mathrm{GeV}$ ) and bottom ( $m_{b}=4.5 \mathrm{GeV}$ ) quarks with $E=15 \mathrm{GeV}$ and virtuality $Q \sim E$ as function of path length. Right panel: The same, but for energies 20 (three upper curves) and 10 GeV (three bottom curves), and zoomed in at short path lengths. and does not radiate any more. Of course, this $b$-quark still may have a medium induced radiation, which is very weak according to 1057 . Notice that the interference between vacuum and induced radiations is absent because they occur on different time scales.
Production and formation length. One should clearly distinguish between the production time scales for a colorless dipole (pre-hadron) and the final hadron. The former signals color neutralization, which stops the intensive energy loss caused by vacuum radiation following the hard process, while the latter is a much longer time taken by the dipole to gain the needed hadronic mass, i.e. to develop the hadron wave function. While the former is proportional to $1-z_{h}$ and contracts at large fractional momentum $z_{h}$ of the hadron, the latter keeps rising proportionally to $z_{h}$. These two time scales are frequently mixed up. The shortness of the production lengths at large $z_{h}$ is dictated by energy conservation. Indeed, a parton originating from a hard reaction intensively radiates, losing energy. This cannot last long, otherwise the parton energy will drop below the energy of the detected hadron. Only the creation of a colorless pre-hadron, which does not radiate gluons any more, can stop the dissipation of energy. Energy conservation thus imposes a restriction on the color neutralization time [1058], $l_{p} \leq \frac{E_{q}}{\langle d E / d z\rangle}\left(1-z_{h}\right)$, which must vanish at $z_{h} \rightarrow 1$. One should also distinguish between the mean hadronization time of a jet, whose energy is shared between many hadrons, and specific events containing a leading hadron with $z_{h} \rightarrow 1$. The production of such a hadron in a jet is a small probability fluctuation, usually associated with large rapidity gap events. The space-time development of such an unusual jet is different from the usual averaged jet. It is illustrated in Fig. 5.76. Notice that one should not mix up the production time with the time scale evaluated in [1059], Eq. (2), which is just the well known coherence time. This is not the time of duration of hadronization which we are interested in. If hadronization were lasting as long as the coherence time, energy conservation would be broken. Besides, a pre-hadron does not have any certain mass, since according to the uncertainty relation it takes time, called formation time, to resolve between the ground and excited states, which have certain masses. Therefore, one cannot evaluate the production time of a pre-hadron relying on the mass of the hadron.

Since the produced pre-hadron strongly attenuates in the nuclear medium, the position of the color neutralization point is crucial for the resulting nuclear suppression. Notice


Figure 5.76. The two-step process of leading hadron production. On the production length $l_{p}$ the quark is hadronizing experiencing multiple interactions broadening its transverse momentum and inducing an extra energy loss. Eventually, the quark color is neutralized by picking up an antiquark. The produced color dipole (pre-hadron) is attenuating in the medium and developing the hadron wave function over the formation path length $l_{f}$.
that such a picture of space-time development of hadronization is classical. In quantum mechanics one cannot say with certainly whether the pre-hadron is produced inside or outside the medium: the inside-outside interference term is significant 1060 .
Heavy flavored hadrons. The production length distribution calculated for light quarks [1052, 1019, 1054 should be similar to that for charm quarks, which have a similar vacuum radiation during the first several fermi. However, a bottom quark, according to Fig. 5.75. dissipates considerably less energy, moreover, its vacuum radiation ceases at the distance of about 1 fm , because the quark completely restores its color field. Of course, confinement does not allow a colored quark, even with a restored field, to propagate freely. It keeps losing energy via nonperturbative mechanisms [1054, like in the string (flux tube) model. Surprisingly, nonperturbative dynamics is more involved into hadronization of heavy compared with light quarks. However, one should remember that this is true only for jets which end up producing leading hadrons with $z_{h} \rightarrow 1$.

A high-energy heavy quark always escapes from the medium and produces an open flavor hadron with no suppression. Therefore, a break-up of a light-heavy dipole propagating in a medium should not lead to a suppression, unless the fractional momentum $z_{h}$ of the detected hadron is fixed at a large value. In such a case, break up of the dipole ignites continuation of vacuum energy loss, which slows down the quark to smaller values of $z_{h}$. This is why a quark should stop radiating at a distance $l \sim l_{p}$ and produce a colorless dipole, which then survives through the medium.

It is interesting that the produced heavy-light, $c-q$ or $b-q$ dipoles expand their sizes faster than a light $\bar{q} q$ dipole. This happens because of the very asymmetric sharing of the longitudinal momentum in such dipoles. Minimizing the energy denominator one gets the fractional momentum carried by the light quark, $\alpha \sim \frac{m_{q}}{m_{Q}}$, which indeed is very small, about 0.1 for charm and 0.03 for bottom. Then according to [1055, 1061, the dipole size is evolving with time as $r_{T}^{2}(t)=\frac{2 t}{\alpha(1-\alpha) E}+r_{0}^{2}$, where $r_{0}$ is the initial dipole separation: the $b-q$ dipole is expanding much faster than $\bar{q} q$.

Conclusions. The hadronization of charm and bottom quarks ends up at a short distance $l_{p}$ with production of a colorless dipole which is strongly absorbed by the medium. This may explain why both of them are strongly suppressed in $A+A$ collisions. Studies of light vs. heavy meson productions at the EIC will clearly be able to validate the discussed effects.

### 5.11 Jets

## Jets, in-medium parton propagation and nuclear gluons

Alberto Accardi, Matthew A. C. Lamont, Gregory Soyez
Preliminary results from the SLAC E665 fixed target experiment have demonstrated jet production in $e+A$ collisions at $s \approx 1000 \mathrm{GeV}^{2}$ [1062, 1063]. Thus, the start of the jet study programme should be feasible in a Phase-I EIC. This can be confirmed by further simulations, required to study the capabilities in a collider experiment as opposed to a fixed-target experiment like E665.

As will be discussed in detail in the next 2 contributions, the nuclear modification of $1+1$ jet production, i.e., 1 jet from current fragmentation and 1 from target fragmentation, is of great interest to study parton propagation through cold nuclear matter, in order to extract cold nuclear transport coefficients, and probing soft gluons in nuclei. In addition, the nucleus can be used as a femtometer-scale detector of the evolution of parton showers, allowing to test their perturbative descriptions (e.g., $k_{T}$-ordering $v s$. rapidity ordering) and Monte-Carlo implementations, which are used pervasively in all fields of high-energy physics to analyze experimental data.

The case of $2+1$ jets is also interesting. Indeed, the cross section for this prcess reads

$$
\begin{equation*}
\frac{\mathrm{d}^{2} \sigma_{2+1}}{\mathrm{~d} x_{p} \mathrm{~d} Q^{2}}=A_{q}\left(x_{p}, Q^{2}\right) q_{A}\left(x_{p}, Q^{2}\right)+A_{g}\left(x_{p}, Q^{2}\right) g_{A}\left(x_{p}, Q^{2}\right) \tag{5.161}
\end{equation*}
$$

where the two terms correspond to the quark-initiated and gluon-initiated processes respectively, and the coefficients $A_{q}$ and $A_{g}$ are matrix elements that can be computed at given order in perturbation theory. Unlike the $1+1$ case which is dominated by quark initiated processes, the $2+1$ cross section is now also sensitive to nuclear gluons, and offers yet another way to measure them.

Since the outgoing jets have to travel in the medium, the coefficients $A_{q}$ and $A_{g}$ will be affected by in-medium propagation. We shall assume here that the measurements of $1+1$ jet cross-sections allow to control in medium quark jets, hence $A_{q}$. Then, by tagging or vetoing gluon jets in $2+1$ events one can study, respectively, gluon jets in-medium propagation and the nuclear gluon distributions. In Fig. 5.77, we show the expected kinematic reach of the gluon measurements for a phase-I and phase-II EIC, and for various cuts on the jet transverse momentum $p_{T}$. Details can be found in [1064. Detailed simulations are planned to study the feasibility and physics reach of these jet studies.

## Monte-Carlo for hard jets in $\mathrm{e}+\mathrm{A}$ collisions

## A. Majumder

The production and modification of hard jets produced in lepton nucleus collisions is considered. The assumption of factorization of the hard scattering cross section from the structure functions and final fragmentation function allow one to compute the final medium modified fragmentation function in both cold nuclear matter and in a hot Quark-GluonPlasma (QGP) in an identical formalism. This allows for both a cross check of the basic energy loss formalism used in these reactions, and a comparative study of the partonic sub-structure of these different phases of QCD matter. Detailed descriptions are provided


Figure 5.77. Left: Parton-level processes that contribute (a) to the $1+1$ and (b,c) $2+1$ jet crosssection. Middle and Center: Accessible kinematic range in $x_{p}$ and $Q^{2}$ for the $2+1$ jets scenario. The accessible region is plotted for different energies $E$ of the electron beam and hadron beam energy $E_{p}=100 \mathrm{GeV}$, corresponding to a phase-I and phase-II EIC, for different jet transverse momentum cuts $p_{T}>p_{T, \text { min }}$ at fixed jet energy cut $E_{c u t}$.
via a Monte-Carlo simulation of such calculations. We compare the results of analytical calculations in these two regimes and present preliminary Monte-Carlo simulations for jets produced in deep-inelastic collisions.
Introduction to in-medium DGLAP. Collision processes which involve a hard scale can be factorized into separate probabilities of hard and soft processes which are convoluted via a single dimensionless variable [716]. For example, for the case of single hadron inclusive production in deep-inelastic-scattering (DIS), the differential cross section may be expressed as,

$$
\begin{equation*}
\frac{d \sigma}{d z}=\int d x G\left(x, Q^{2}\right) \otimes \frac{d \hat{\sigma}}{d Q^{2}} \otimes D\left(z, Q^{2}\right) \tag{5.162}
\end{equation*}
$$

where, $G\left(x, Q^{2}\right)$ represents the parton distribution function, $\frac{d \hat{\sigma}}{d Q^{2}}$ represents the electron quark scattering cross section via single photon exchange. $D\left(z, Q^{2}\right)$ represents the fragmentation function to produce a hadron with a momentum $z \nu$ from the fragmentation of the outgoing quark jet. The structure functions and fragmentation functions are defined and factorized from the hard cross sections at a given scale $\mu^{2}$ which, in this case, is chosen to be equal to the hard scale of the process $Q^{2}$. They only need to be measured at a single scale, and the change of these functions with scale is given by the DGLAP evolution equations 856. For fragmentation functions, these equations read

$$
\begin{equation*}
\frac{\partial D\left(z, Q^{2}\right)}{\partial \ln Q^{2}}=\frac{\alpha_{S}}{2 \pi} \int \frac{d y}{y} P(y) D\left(\frac{z}{y}, Q^{2}\right), \tag{5.163}
\end{equation*}
$$

where, $P(y)$ is the gluon splitting function and represents the probability for a quark to radiate a gluon and retain a fraction $y$ of its light cone momentum.

In the case of DIS on a large nucleus, one may simply include the entire effect of the medium by including a length dependent multiplicative factor to the gluon splitting function [1065], which accounts for the fact that the radiated gluon will scatter in the medium influencing its radiation amplitude, i.e., $P(y) \rightarrow P(y) K\left(y, q^{-}, L^{-}, Q^{2}\right)$. The medium dependent factor given as [1066],

$$
\begin{equation*}
K\left(y, q^{-}, L^{-}, Q^{2}\right)=\int_{0}^{L^{-}} d \zeta^{-} \frac{\hat{q}}{Q^{2}}\left[2-2 \cos \left(\frac{Q^{2} \zeta^{-}}{2 p^{+} q^{-} y(1-y)}\right)\right] \tag{5.164}
\end{equation*}
$$



Figure 5.78. Left: A comparison of the results of an analytic DGLAP evolution calculation and a Monte-Carlo shower calculation for the same choice of input parameters. Right: Results of a set of Monte-Carlo simulations of a jet propagating through a 4 fm brick.

In the equation above, $L^{-}$is the maximum possible length traversed in the medium in the course of one emission. In an evolution equation, the formation time of the final radiation is chosen to be larger than the maximum medium length. This restricts the length to be no larger than $q^{-} / Q_{\min }^{2}$, where $Q_{\text {min }}$ is the minimum allowed virtuality on exit from the medium. In an analytic solution to the DGLAP equation, one requires an input fragmentation function. The most unambiguous input is to use the known vacuum fragmentation function at the scale $Q_{\min }^{2}$ where we have stipulated that the jet has emerged from the medium. This is then evolved in $Q^{2}$ up to the hard scale of the process using the medium modified evolution equation which includes the kernel of Eq. (5.164).

Results from such an in-medium DGLAP evolution are plotted in Fig. 5.78. The input distribution in vacuum is taken from KKP at an input scale of $\mu_{i n}^{2}=1 \mathrm{GeV}^{2}$ and evolved up to $Q^{2}$. Its ratio to the KKP fragmentation at the scale $Q^{2}$ is plotted as the green dashed line in Fig. 5.78, Note that our numerical implementation of the DGLAP equation is different from that of KKP and so for comparison, we plot the ratio of the vacuum evolved fragmentation function in our implementation versus that in the KKP where both calculations start from the same input distribution i.e. the KKP function at the scale $\mu_{i n}^{2}$, and are compared at the higher scale of $Q^{2}$. The ratio is plotted as the magenta curve in Fig. 5.78, While over the range of $z$ considered, the curve is close to unity, it may deviate by up to $20 \%$ at lower values of $z$.

The solid blue line in Fig. 5.78 represents the ratio of the medium modified fragmentation function to the vacuum fragmentation function, where both numerator and denominator are calculated using the same numerical routine (for the vacuum FF we simply use $\hat{q}=0$ ). This ratio can be approximately compared to the ratio of hadron yields in DIS experiments. It should be pointed out that in all the calculations reported in this article, the medium is assumed to be static and uniform with a fixed length. This fixed length is travelled by each jet. Realistic geometries will be considered in the future.
Monte-Carlo implementation. In any realistic calculation of jet modification in an extended medium a variety of approximations need to be made. For example, in the inmedium DGLAP evolution equations reported in the previous sections, we assumed that
the entirety of the parton shower exits the medium and fragments in vacuum. This is obviously not the case. In reality, a large portion of the shower is trapped in the medium and does not undergo vacuum fragmentation. Such effects cannot be treated in a DGLAP setup where the input is the final vacuum fragmentation. Note that such effects may be included with a position dependent input fragmentation function. However, such input is always ambiguous and the computation of the evolution of a position, energy and obviously $z$-dependent fragmentation functions are prohibitively numerically intensive.

The obvious solution to this is to use a Monte-Carlo jet routine. Unlike analytic inmedium DGLAP calculations which evolve upwards, numerical Monte-Carlo routines evolve downwards in virtuality. As such, they are a more natural calculation which reconstructs the shower forwards in time. One starts with the original produced hard virtual parton and then constructs the Sudakov factor

$$
\begin{equation*}
\Delta\left(Q^{2}, \mu^{2}\right)=\exp \left[-\frac{\alpha_{S}}{2 \pi} \int_{\mu^{2}}^{Q^{2}} \frac{d q^{2}}{q^{2}} \int d y P(y)\left\{1+K\left(y^{-}, q^{-}, L^{-}, q^{2}\right)\right\}\right] \tag{5.165}
\end{equation*}
$$

which yields the probability of no resolvable emission between $Q^{2}$ and $\mu^{2}$ and uses this to numerically estimate the probability of the initial parton being produced with a maximum virtuality of $\mu^{2}$. One then samples the splitting function to estimate the probability that the produced partons have fractions $y$ and $1-y$ of the parent parton. Unlike the case of the vacuum Sudakov factor, the equation above also contains in addition the medium dependent kernel $K$ defined in Eq. (5.164). This means that at each point, the shower may undergo either a vacuum split or a medium induced split. It also clearly demonstrates how the probability of splitting increases in the medium. At each point, we estimate the location of the parton based on its formation time, which may be easily obtained from its virtuality and its energy.

This showering routine is repeated to obtain partons with lower and lower virtuality. We terminate the shower when the virtuality of the parton reaches $\Lambda_{0}=1 \mathrm{GeV}$. If at this point the parton is found outside the medium, then it is convoluted with a vacuum fragmentation function. If it is found inside the medium then it is removed from the final shower. We point out again that the medium in all these calculations is not a real nucleus, but rather a static brick. Once the shower is calculated in the medium, it is then repeated in vacuum. Thus, both numerator and denominator of the ratio of fragmentation functions are calculated by an identical routine.

Using this implementation we may repeat our calculations in the HERMES-like systematics of Fig. 5.78, The results of the Monte-Carlo is represented by the solid black line. We should mention in passing that the fragmentation function used in the Monte-Carlo calculation is BKK while that in the DGLAP is KKP. We note that the ratio of fragmentation functions are rather similar. The Monte-Carlo results are for the most part below the DGLAP calculation. This is because of the mechanism by which we can systematically remove the partons which fragment in the medium, which can only be done in the MC calculation. The excess at lower $z$ is partially due to the use of a different fragmentation function and partially due to some of these partons having a long formation time.

Having tested the Monte-Carlo calculation in HERMES-like systematics ( $E=20 \mathrm{GeV}$ and $Q^{2}=3 \mathrm{GeV}^{2}$ ), we apply the MC calculation to the EIC-like systematics ( $E=25,35,50$ GeV and $Q^{2}=100 \mathrm{GeV}^{2}$ ). First off, we note that even with the larger energies there is a considerable amount of suppression. This is due to the larger $Q^{2}$ of the produced jet. Such jets tend to shower a lot and thus end up being considerably affected by the medium. This
goes beyond what is known at HERMES that increasing the energy reduces the observed suppression. We also find a kind of universal suppression at large $z$ which is independent of energy. This kind of universal suppression was also noted in the DGLAP calculations performed for comparison with the HERMES data. In the earlier DGLAP calculations, the reason for the scaling was due to the vanishing of the real part of the evolution equation, leaving the same virtual corrections for different energies. It is difficult to state at this point if the scaling observed in the Monte-Carlo calculations is due to a similar reason, i.e., the vanishing of the real part of the equivalent DGLAP calculation.

If the results reported here are verified by a future EIC, this would represent an interesting observation: to find an almost $50 \%$ suppression in the large $z$ yield even for 50 GeV jets. Such high $Q^{2}$ jets should be describable using perturbation theory over a large part of their lifetime and would thus yield deep probes of the medium through which they propagate. This would allow for a much clearer understanding of the gluonic structure of nucleons inside nuclei. It would also greatly facilitate our understanding of how jets are modified in a dense extended environment, which would allow for more refined probes of matter produced in heavy-ion collisions.

## Jet evolution in hot and cold matter

## Hans J. Pirner

We will discuss jet propagation in hot matter first before addressing jet propagation in the "cold" matter of electron-nucleus collisions. A common interpretation of the large pion attenuation in $\mathrm{Au}+\mathrm{Au}$ collisions at RHIC is parton energy loss, where hadronization occurs outside of the hot zone and is not affected by the medium. There is no doubt that gluon radiation plays an important role for the energy loss and the parton evolution at RHIC and the LHC. The respective virtualities of partons are around $Q=20 \mathrm{GeV}$ and $Q=100 \mathrm{GeV}$. In our modeling of jet evolution [1067, 1068] the parton shower is treated together with the propagation of the parton in the medium which is more realistic because of the relevant time scales. A typical shower at RHIC lasts about $\tau_{\text {evo }}=2 \mathrm{fm}$. The non-perturbative part of hadronization involves the decay of the resonances at the pre-confinement scale $Q_{0}=1-2 \mathrm{GeV}$ into $3-4$ pions. The lifetime of the plasma can be estimated at $\tau_{c}=3.3 \mathrm{fm}$. Comparing the two time estimates, we see that at the end of the evolution at RHIC, resonances interact with hadronic resonance matter. This process can be described by a hadronic theory with cross sections slightly larger than hadronic cross sections in vacuum. Because of these large cross sections, absorptive effects play a decisive role in the observed suppression of hadrons in RHIC experiments. We have advocated two scenarios. Scenario 1 uses the conservative radiative energy loss obtained from QCD and includes pre-hadron formation and resonance absorption. Scenario 2 neglects the resonance phase but tunes up the energy loss parameter to fit the data.

In more detail, our model [1067] works as follows: The parton produced in a hard process radiates successively to reduce its virtuality and become on mass-shell. This parton shower is modified by scattering in the medium. As both terms enter the same equation, one cannot separate scattering and radiation. This equation includes truly radiative energy loss, but without coherence. Quark fragmentation at RHIC and gluon fragmentation at the LHC should give the essential results. The indices on the fragmentation functions and the splitting functions can then be dropped and the formalism becomes simpler. For the in-medium fragmentation function $D^{m}\left(x, Q^{2}\right)$ we include into the DGLAP evolution the
scattering term $S\left(x, Q^{2}\right)$.

$$
\begin{equation*}
\frac{\partial D^{m}\left(x, Q^{2}\right)}{\partial \ln Q^{2}}=\frac{\alpha_{s}\left(Q^{2}\right)}{2 \pi} \int_{x}^{1} \frac{\mathrm{~d} z}{z} P(z) D^{m}\left(\frac{x}{z}, Q^{2}\right)+S\left(x, Q^{2}\right) \tag{5.166}
\end{equation*}
$$

with

$$
\begin{equation*}
S\left(x, Q^{2}\right) \simeq f \frac{n_{g} \sigma\left\langle q_{\perp}^{2}\right\rangle}{2 m_{s} Q^{2}}\left(D\left(x, Q^{2}\right)+x \frac{\partial D}{\partial x}\left(x, Q^{2}\right)\right) \tag{5.167}
\end{equation*}
$$

The quantity appearing in the scattering term is the jet transport parameter $\hat{q} \simeq \bar{n} \bar{\sigma}\left\langle q_{\perp}^{2}\right\rangle$, which describes the mean acquired transverse momentum of the parton per unit length.

To allow a direct fit of experimental data with only parton energy loss, we introduce a possible enhancement factor $f$ in the scattering term. The scattering term is most relevant at small virtualities $Q \simeq Q_{0}$ and consequently we have used the scale $Q_{0}$ in $\alpha_{s}$ to arrive at an upper boundary for $\hat{q}$. More explicitly, these expressions give $\hat{q}=0.5 \mathrm{GeV}^{2} / \mathrm{fm}$ for a temperature of $T=0.3 \mathrm{GeV}$ for RHIC and $\hat{q}=5.2 \mathrm{GeV}^{2} / \mathrm{fm}$ for $T=0.5 \mathrm{GeV}$ corresponding to the LHC. As shown in ref. 1067 we can fit the RHIC data including prehadron absorption in the final state resonance gas. The prediction for LHC gives $R_{A A} \approx 0.4$. If we use an enhancement factor $f=8$ which is beyond any higher order QCD correction, the measurement of hadrons with high transverse momentum would be totally suppressed at the LHC.

Let us now discuss jets in cold matter resulting from DIS on nuclei. Electron scattering on a target at intermediate Bjorken $x$ can be treated along similar lines as the DGLAP evolution of the quark jet in the cold medium, whereas electron-nucleus scattering at low $x$, in principle necessitates the evolution of the quark and antiquark produced from photongluon fusion. It is not clear whether the cascades from the two reaction products behave independently when they propagate through the target. In the Ariadne model, two strings result from the quark and antiquark produced by photon-gluon fusion. The first string connects the antiquark with the quark which emitted the gluon. The second string combines the quark with the remnant di-quark of the proton. Due to the aligned jet configuration, one of the two strings only contains a few low momentum particles and perhaps may be neglected in the first approximation. The evolution equation outlined above can then be applied to jet propagation in cold matter, and applications to an EIC are planned. Scattering partners of the quark are nucleons and the quantity $<\sigma q_{\perp}^{2}>$ can be derived from the dipole cross section on nucleons. The resulting transport parameter at HERMES energies is very small $\hat{q}=0.035 \mathrm{GeV}^{2} / \mathrm{fm}$ and has been tested in hadronic broadening of the produced hadrons [1069]. For a high energy machine with an electron-nucleon energy $E_{c m}=100 \mathrm{GeV}$ the transport parameter will be larger due to the increasing dipole cross section, we estimate that the transport parameter will increase to about $\hat{q}=0.1 \mathrm{GeV}^{2} / \mathrm{fm}$. So effects should well be observable, but smaller than at RHIC.

### 5.12 Target fragmentation

## Fragmentation of nuclei - a critical tool for novel QCD phenomena

Mark Strikman

The main focus of the discussions on quark propagation through the nucleus has been on current fragmentation processes, e.g., the suppression of the leading hadron spectrum, $p_{t}$ broadening and jet propagation in nuclear matter. So far, very little attention has been paid to nuclear fragmentation in DIS. To some extent, this is due to the lack of experimental data as such measurements are very challenging. However, while nuclear effects in the current fragmentation region decrease with increasing $Q^{2}$ at fixed $x$, the nuclear effects in the fragmentation region persist in this limit, and are likely to depend on $x$. They may help address a number of important questions:

- Are color tubes formed in propagation of quarks through nuclear media?
- How different are the propagations of gluons and quarks through the nuclear media?
- How different are the propagations of quark and dipole?

To visualize these questions, it is convenient to consider the process in the nuclear rest frame and distinguish three kinematic regions: (a) For $x \geq 0.1$, a quark is knocked out (or a gluon if we consider for example a leading di-jet or charm production in DIS), (b) for $0.1>x \geq 1 /\left(2 R_{A} m_{N}\right)$ the virtual photon converts to a $q \bar{q}$ pair inside a heavy nucleus, and (c) for $x<1 / 2 R_{A} m_{N}, \gamma^{*} \rightarrow q \bar{q}$ transition occurs predominantly before the target, see Fig. 5.79

In the case of of $x>0.1$ and large $Q^{2}$ corresponding to the knock out of a quark, a color triplet $q q$ system is left inside the nucleus and it is typically moving along the virtual photon momentum direction with a relatively small velocity. The knocked out quark fragments into partons/hadrons at longitudinal distances $y \geq 2 p_{q} / \Delta m^{2} \gg R_{A}$, where $\Delta m^{2} \sim 1 \mathrm{GeV}^{2}$ can be estimated based on the current DIS data [1014]. It is similar to that for color transparency processes. As a result, the leading hadron spectrum at large $Q^{2}$ approaches the universal limit given by pQCD. This pattern is consistent with the experimental data. Different to the naive expectations of the parton model, an A-dependent $p_{t}$ broadening in present in this limit. Naively the hadrons produced in the fragmentation of the quark are formed at distances given by $y \geq 2 p_{h} / \Delta m^{2}$, so that there should be a depletion in the spectrum at $p_{h}^{\text {crit }} \sim \Delta m^{2} R_{A} / 2$ followed by an enhancement at rapidities close to the nuclear rapidity (hadron pileup). Since for heavy nuclei $p_{h}^{\text {crit }} \sim 10 \div 20 \mathrm{GeV} / \mathrm{c}$, one would expect a strong deformation of the hadron spectrum with a large increase of multiplicity for $\left|y-y_{A}\right| \leq 2 \div 3$ for $A \sim 200$. In particular, it would be manifested in the strong break up of the heavy


Figure 5.79. Space-time picture of DIS in the nucleus rest frame for different x


Figure 5.80. Left: Coulomb exchanges may lead to formation of extended spatial regions where color is not screened. Right: The E665 data 1070 for the soft neutron multiplicity compared with the calculation of 1071.
nuclei which is associated with emission of many soft neutrons. One should also expect an increase of the multiplicity of soft neutrons with an increase of $p_{t}$ of the leading hadron, since large $p_{t}$ selects events with extra Coulomb exchanges which are more likely for longer quark paths inside the nucleus and should result in a larger number of wounded nucleons. These may also lead to the creation of large unscreened color regions in the nucleus - see Fig.5.80. An open question is how these expectations could be affected by a high degree of coherence in the emission of the partons in pQCD. Such a coherence may lead to strong screening effects in the formation of the final state and in particular a reduction of $\Delta m^{2}$ away from the current fragmentation region. Also, if the color tube is very narrow, a chance that the tube intersects with other nucleons maybe significantly reduced.

For intermediate $x \sim 0.05$, the virtual photon also penetrates any point in the nucleus but it can hit either quark or antiquark, so in principle, by studying the properties of the leading hadron one can compare the structure of the final state interaction for the removal of quark and antiquark which maybe different, for example since $\bar{q}$ can belong to a color singlet $q \bar{q}$ cluster.

For small $x \leq 0.03$, the virtual photon predominantly transforms into a $q \bar{q}$ pair before the target nucleus. In the aligned jet model one would expect that the number of wounded nucleons would be given by $A \sigma(e N) / \sigma(e p)$ with the hadrons formed at the similar distances as in the large $x$ case. Hence naively one would expect that many nucleons will be wounded in a heavy nucleus, leading to a strong excitation of the nucleus which is known to be associated with multiple neutron emission, and emission of protons with momenta of $\geq 300$ $\mathrm{MeV} / \mathrm{c}$, see also Section 5.12.

The process of neutron emission in DIS off Pb was studied by the E665 collaboration at FNAL for average $x \sim 0.05$ and $Q^{2} \sim$ few $\mathrm{GeV}^{2} 1070$. The results of the measurement are compared the theoretical calculation of [1071] in Fig. 5.80. Calculations using a Monte Carlo event generator tuned to reproduce the neutron emission in the proton-nucleus scattering reproduces both the neutron multiplicity and the neutron momentum distribution, provided only recoil nucleons with energy smaller than 1 GeV are allowed to interact in the nucleus. Taken at face value, this suggests a very strong reduction of the final state interactions at large energies which is consistent with the trend of the E665 data to have a smaller neutron multiplicity for larger $\nu$.

At very small $x$ and moderate $Q^{2}$, one may reach the black disk regime. In this regime, the leading hadron spectrum is reduced and the pQCD factorization for the parton fragmen-
tation breaks down in a gross way [981, see also Section 5.8. In this limit, the selection of events with enhanced activity in the nuclear fragmentation region should lead to reduction of the forward spectrum: this would provide a clear signal for a new regime, since no such correlation is possible in the leading-twist pQCD regime.

In summary, hadron production in the nuclear fragmentation region is very sensitive to the dynamics of space-time evolution of the triplet and octet color tubes as well as of color dipoles. This is one of the unexplored frontiers where the collider kinematics will allow a qualitative improvements in the data, and likely lead to the discovery of a series of new regularities. This may include a much higher degree of coherence in the fragmentation (hinted at by the E665 data) than suggested by the current models. Understanding of the fragmentation dynamics will be also of great help for understanding the dynamics in the nuclear fragmentation region in heavy ion collisions, where high density quark-gluon systems may be produced.

## In-medium hadronization and EMC effects in nuclear SIDIS

C. Ciofi degli Atti, L. P. Kaptari, B. Z. Kopeliovich, and C. B. Mezzetti

The SIDIS process $A\left(e, e^{\prime}(A-1)\right) X$ in which, instead of the leading hadron, a nucleus ( $A-1$ ) in the ground or in low excitation states is detected in coincidence with the scattered electron, can provide new information about the mechanism of hadronization and the origin of the EMC effect [1072, 1073, 1074, 1075, 1076]. Two main advantages of the new SIDIS process over the classical SIDIS [1010] and inclusive $A\left(e, e^{\prime}\right) X$ scattering [1077] are worth mentioning here. Firstly, it can provide a new insight into the space-time development of hadronization at the early stage, which can be probed only by placing additional scattering centers at microscopic distances, i.e. by using nuclear targets. By detecting a jet produced on a nuclear target, one can get information about its time development, but in a rather indirect and complicated way, since cascading inside the nuclear medium essentially modifies the observables. Measuring the recoil nucleus supplies additional and cleaner information about the dynamics of hadronization; in particular, this process is free of the uncertainties caused by cascading, and the survival probability of the recoil nucleus is extremely sensitive to the multiparticle components of the jet [1072. Secondly, a proper ratio of the cross sections on a nucleus $A$ taken at different values of the Bjorken scaling variable $x_{B j}$ provides information on the nucleon structure functions in the medium, $F_{2}^{N / A}$. Several experimental projects to investigate the new process at 12 GeV have been proposed thanks to the development of proper recoil detectors [1078], and the experiment on Deuteron targets has already been performed [1079].

The basic ingredients of the theoretical calculation are the nuclear momentum distributions, the nucleon structure function $F_{2}^{N / A}$ in the medium, and the effective cross section of interaction between the hadronizing nucleon debris and the spectator nucleons. This last reads 1072

$$
\begin{equation*}
\sigma_{e f f}\left(z, x_{B j}, Q^{2}\right) \equiv \sigma_{e f f}(z)=\sigma_{t o t}^{N N}+\sigma_{t o t}^{\pi N}\left[n_{M}(z)+n_{G}(z)\right] \tag{5.168}
\end{equation*}
$$

where $\sigma_{\text {tot }}^{N N}$ and $\sigma_{\text {tot }}^{\pi N}$ are the total nucleon-nucleon $(N N)$ and pion-nucleon $(\pi N)$ cross sections, and the $Q^{2}$ - and $x_{B j}$-dependent quantities $n_{M}(z)$ and $n_{G}(z)$ denote the pion multiplicities due to the breaking of the color string and to gluon radiation, respectively. Their explicit form directly follows from the hadronization mechanism proposed in Ref. [1080], leading to a satisfactory description of the grey track production in DIS off nuclei [1032].


Figure 5.81. Top panels: the distorted momentum distributions $n_{0}$ with $\theta=\widehat{\theta_{\mathbf{P}_{A-1} \mathbf{q}}}$ and $p \equiv\left|\mathbf{P}_{A-1}\right|$ for ${ }^{3} \mathrm{He}$ and ${ }^{40} \mathrm{Ca}$. Bottom panels: The ratio $R\left(A, A^{\prime}\right)$ of Eq. 5.171 with $A=2$, and $A^{\prime}={ }^{3} \mathrm{He}$ or ${ }^{40} \mathrm{Ca}$.

The cross section of the $A\left(e, e^{\prime}(A-1)\right) X$ process [1072, 1074] schematically reads

$$
\begin{equation*}
\frac{d \sigma^{A, F S I}}{d x_{B j} d Q^{2} d \mathbf{P}_{A-1}}=F_{2}^{N / A}\left(x_{A}, Q^{2}, k^{2}\right) \otimes n_{0}^{A, F S I}\left(\mathbf{P}_{A-1}\right) \tag{5.169}
\end{equation*}
$$

where $x_{A}=x_{B j} / z_{1}^{(A)}, z_{1}^{(A)}=\left(M_{A} k \cdot q\right) /\left(m_{N} P_{A} \cdot q\right), k$ is the four-momentum of the bound nucleon and $P_{A}$ of the target nucleus. In this equation, $n_{0}^{A, F S I}\left(\mathbf{P}_{A-1}\right)$ is the distorted momentum distribution of the bound nucleon after final state interaction (FSI) with the debris nucleon ( $\mathbf{k}_{1}=-\mathbf{P}_{A-1}$ in Plane Wave Impulse Approximation):

$$
\begin{equation*}
\left.n_{0}^{A, F S I}\left(\mathbf{P}_{A-1}\right)=\frac{1}{2 J_{A}+1} \sum_{\mathcal{M}_{A}, \mathcal{M}_{A-1}}\left|\int d \mathbf{r}_{1}^{\prime} e^{i \mathbf{P}_{A-1} \mathbf{r}_{1}^{\prime}}\left\langle\Psi_{J_{A-1}, \mathcal{M}_{A-1}}^{0}\right| S_{F S I}^{X N}\right| \Psi_{J_{A}, \mathcal{M}_{A}}^{0}\right\rangle\left.\right|^{2}(5 \tag{5.170}
\end{equation*}
$$

where $S_{F S I}^{X N}$ is the debris-nucleon eikonal scattering $S$-matrix which differs from the Glauber form because of the $z$ dependence of $\sigma_{e f f}$ [1081]. The results of some calculations are presented in what follows, using for Deuteron and ${ }^{3} \mathrm{He}$ realistic wave functions [1082] corresponding to the AV18 interaction [1083], and for heavy nuclei single particle mean field wave functions. A good agreement between our parameter-free calculation [1076] and the experimental data for $2 H\left(e, e^{\prime} p\right) X$ around $\theta \simeq 90^{\circ}$ is exhibited.

The distorted momentum distributions of ${ }^{3} \mathrm{He}$ and ${ }^{40} \mathrm{Ca}$ at kinematics more appropriate for an EIC are shown in Fig. 5.81, As already pointed out, the FSI is governed by the details of $\sigma_{e f f}$ and strongly affects the survival probability of $(A-1)$, as it can be seen by comparing the results for ${ }^{3} \mathrm{He}$ and ${ }^{40} \mathrm{Ca}$. Let us denote the cross section (5.169) by $\sigma^{A, F S I}$. Then, if our description is correct, the ratio of cross sections on different nuclei,

$$
\begin{equation*}
R\left(A, A^{\prime}, \mathbf{P}_{A-1}\right)=\frac{\sigma^{A, \exp }\left(x_{B j}, Q^{2},\left|\mathbf{P}_{A-1}\right|, z_{1}^{(A)}, y_{A}\right)}{\sigma^{A^{\prime}, \exp }\left(x_{B j}, Q^{2},\left|\mathbf{P}_{A-1}\right|, z_{1}^{\left(A^{\prime}\right)}, y_{A^{\prime}}\right)} \rightarrow \frac{n_{0}^{(A, F S I)}\left(\mathbf{P}_{A-1}\right)}{n_{0}^{\left(A^{\prime}, F S I\right)}\left(\mathbf{P}_{A-1}\right)} \tag{5.171}
\end{equation*}
$$

should be governed only by the FSI, as shown in Fig. 5.81.


Figure 5.82. The ratio $R\left(x_{B j}, x_{B j}\right)$ of Eq. (5.172) for the process ${ }^{3} H e\left(e, e^{\prime} d\right) X$ and ${ }^{40} C a\left(e, e^{\prime 39} K\right) X$ calculated with different nucleon structure functions: i) free structure function; ii) off mass-shell (xrescaling) structure function; iii) with suppression of point-like configurations (PLC) in the medium depending upon the nucleon virtuality 1084$]\left(P_{A-1} \equiv\left|\mathbf{P}_{A-1}\right|\right)$.

In order to tag bound nucleon structure functions, whose nuclear modification is one of the causes of the EMC effect, one has to get rid of the distorted nucleon momentum distributions and other nuclear structure effects. This can be achieved by considering the ratio of the cross sections on a nucleus $A$ measured at two different values of the Bjorken scaling variable, $x_{B j}$ and $x_{B j}^{\prime}$, leaving unchanged all other quantities in the two cross sections, i.e., the ratio

$$
\begin{equation*}
R\left(x_{B j}, x_{B j}^{\prime},\left|\mathbf{P}_{A-1}\right|\right)=\frac{\sigma^{A, \exp }\left(x_{B j}, Q^{2},\left|\mathbf{P}_{A-1}\right|, z_{1}^{(A)}, y_{A}\right)}{\sigma^{A, \exp }\left(x_{B j}^{\prime}, Q^{2},\left|\mathbf{P}_{A-1}\right|, z_{1}^{(A)}, y_{A}\right)} \approx \frac{F_{2}^{N / A}\left(x_{A}, Q^{2}, k^{2}\right)}{F_{2}^{N / A}\left(x_{A}^{\prime}, Q^{2}, k^{2}\right)} \tag{5.172}
\end{equation*}
$$

which depends only upon the nucleon structure function $F_{2}^{N / A}$. Calculations of the ratio (5.172) have been performed [1076] using three different structure functions, namely, the free one, giving no EMC effect, and two medium dependent structure functions, yielding only a few percent difference in the inclusive cross section. It can be seen from Fig. 5.82 that the discrimination of different models of the medium dependence of $F_{2}^{N / A}\left(x_{A}, Q^{2}, k^{2}\right)$ can indeed be achieved, especially at large $P_{A-1} \equiv\left|\mathbf{P}_{A-1}\right|$.

In conclusion, from what shown here and in the original papers [1073, 1072, 1074, 1075, 1076 it appears that the SIDIS process $A\left(e, e^{\prime}(A-\right.$ 1)) $X$, with detection of a complex nucleus $(A-$ 1), would be extremely useful to clarify the origin of the EMC effect and to study the early stage of hadronization at short formation times. At EIC kinematics (large $Q^{2}$ and $W_{X}^{2}$ ), the


Figure 5.83. The production cross section of neutrons with low momenta for different longitudinal production points, normalized to the corresponding number of events. (The calculations are preliminary.) theoretical assumptions underlying Eqs.(55.168)(5.170) are expected to be of higher validity than at lower energy. The problem remains as to whether experiments of the kind we are discussing, i.e. the detection of low-momentum light nuclei at specific angles, could be performed at an Electron Ion Collider. We have calculated the process ${ }^{3} \mathrm{He}\left(e, e^{\prime} d\right) X$ at various EIC kinematics and found that, e.g. at $Q^{2} \simeq 30 \mathrm{GeV}^{2}$ and $x_{B j} \simeq 0.7$, when the Deuteron is emitted at about $90^{\circ}$ in the target
rest frame, this corresponds to about $1^{0}$ in the direction of the incident nucleus in the collider CM frame.

## Proving the microscopic origin of nuclear forces

## Mark Strikman

An important task for the EIC is to probe nuclear forces on the microscopic level using hard probes. Before describing some of the possible avenues for EIC research, it is worth summarising what is already known from the analyses of the experimental studies of the nuclear pdfs.

- The quark distributions at large $x$ are suppressed as compared to the naive expectations based on the picture of the nucleus built of nucleons with internal parton distributions coinciding with the free nucleon pdfs, the so called EMC effect - for a review see e.g. [942. However, the EMC effect modification of the nucleon pdfs remains small - $\leq 2 \%$ for $x \leq 0.5$ after one takes into account the Coulomb field contribution into the wave function of the heavy nuclei and uses the proper scaling variable $x_{A}=A Q^{2} / 2 q_{0} M_{A}$ for the comparison of the nuclear cross sections [1085]. The modification of the nucleon pdfs strongly grows with $x$ at $x>0.5$ reaching $\sim 10 \%$ at $x=0.6$.
- The $A$-dependence of the EMC effect at large $x$ indicates that the main contribution to the EMC effect is due to scattering off the short-range correlations (SRC) in nuclei.
- Experiments at JLab confirm approximate $A$-independence of the momentum distribution of nucleons in the short-range correlations, though the absolute probability is a factor of $\sim 5$ larger in heavy nuclei than in the deuteron, for a recent review see [1086.
- The measurements of the antiquark distributions in nuclei were performed using the Drell-Yan process. No enhancement of the $\bar{q}_{A} / \bar{q}_{N}$ ratio was observed for $x \sim 0.1$ where the models of nuclear forces with dynamic pion fields predicted $10 \div 20 \%$.
- Application of the baryon and momentum sum rules indicate that the valence quarks and gluons are enhanced in nuclei at $x \sim 0.1$ [1087, 828].

The region of $x \sim 0.1$ is especially interesting for the purposes of studying the QCD origin of the nuclear forces since it corresponds to the Ioffe distances $\sim 1 / 2 x m_{N} \sim 1 \mathrm{fm}$, characteristic of more medium and short-distance nuclear forces. The regularities listed above suggest that meson exchanges which lead to the enhancement of the sea quark distributions are less important than it is suggested in the meson models of the nuclear forces, while quark and gluon interchanges between nearby nucleons play a significant role. The inclusive measurements at the EIC will directly measure $V_{A} / V_{N}, G_{A} / G_{N}$ for $x \sim 0.1$.

A new tool which will be available at the EIC is exclusive hard processes for which the QCD factorization theorem has been proven for the processes $\gamma_{L}+T \rightarrow V M+T^{\prime}$ for the Bjorken limit and the mass of the final system $T^{\prime}$ being fixed [572]. We will focus on the processes with deuteron target since in this case it is easier to select scattering off the compact proton - neutron configurations and measure a complete final state. The rational here is that the structure of the SRC in nuclei is approximately the same while using a
heavier target, say ${ }^{4} \mathrm{He}$ would increase the impulse approximation interaction rate by a factor of $\sim 3$ only (due to a higher probability of SRCs in ${ }^{4} \mathrm{He}$ ). However this apparent gain will be compensated to a large extent by the final state absorption/distortions and multistep processes significantly complicating the interpretation of the observations.

The first question one can address is whether the quark and gluon transverse distributions in bound nucleon are the same. The simplest possible processes are break up of the deuteron

$$
\begin{equation*}
\gamma+{ }^{2} H \rightarrow J / \psi+p+n . \tag{5.173}
\end{equation*}
$$

and

$$
\begin{equation*}
\gamma_{L}^{*}+{ }^{2} H \rightarrow \rho^{-}+p+p . \tag{5.174}
\end{equation*}
$$

which probe gluon and quark transverse distributions.
The exclusivity of the process could be tested by measuring $p_{t}\left(N_{1}\right)+p_{t}\left(N_{2}\right)+p_{t}(V M)=$ 0 . To avoid an ambiguity which of the nucleons was interacting via the hard process $\gamma^{*}+N \rightarrow V M+N$, one needs to select transverse momenta of the vector meson $\geq 600 \div$ $700 \mathrm{MeV} / \mathrm{c}$ with momentum of the nucleon $N_{1}$ in approximately the opposite direction. For the spectator to belong to the SRC one needs to ensure that it has a large momentum in the deuteron rest frame $\geq 0.3 \mathrm{GeV} / \mathrm{c}$. It could be either mostly longitudinal or have a transverse component sufficiently deviating from the direction opposite to $p_{t}(V M)$.

The measurement involves studying the dependence of the ratio of the cross section of the reaction (5.173), (5.174) and elementary reaction

$$
R\left(p_{s} p\right)=\frac{\frac{d \sigma\left(\gamma^{*}+{ }^{2} H \rightarrow N N+V M\right)}{d W_{\gamma N} d Q^{2} d t, d p_{s p}}}{\frac{d \sigma\left(\gamma^{*}+N \rightarrow N+V M\right)}{d W_{\gamma N} d Q^{2} d t}}
$$

on the momentum transfer to the vector meson $-t \approx-p_{t}(V M)^{2}$ for fixed values of $p_{s p}$. Deviations of the t -dependence from a constant (which can be calculated in the two nucleon approximation) would signal the change of the size of the bound nucleon. The theoretical expectation is that such effects are proportional to the nucleon "off-shellness" so they should rapidly increase with increasing $p_{s p}$, roughly $\propto p_{s p}^{2}$ [1088, 1084]. It is worth noting that nucleon deformation along and transverse to the direction between the nucleons may differ (like in the case of polarization of the atoms in the molecules). Hence a nontrivial dependence of $R\left(p_{s} p\right)$ on the angle between $p_{s p}$ and $p_{t}(V M)$ is possible (such a dependence is absent if the deformation depends only on the virtuality). It would be possible to study the dependence of $R\left(p_{s} p\right)$ on $x$ (for photoproduction of $J / \psi$ on $m_{J / \psi}^{2} / W^{2}$ probing how the nucleon deformation depends on $x$ of the gluon in the bound nucleon wave function.

Another possible direction for studies is probing directly the pion exchange mechanism using exclusive hard processes - for example $\gamma+{ }^{2} H \rightarrow J / \psi+\pi^{-}+p p$ with transverse momenta of $J / \psi$ and $\pi^{-}$back to back and large deuteron rest frame momenta of both protons (to ensure that the process occurs off the SRC).

The discussed class of the reactions is well suited also for looking for non-nucleonic baryonic components in the SRCs (six quarks, $\Delta \Delta, \ldots$ ). For example one can study the process $\gamma+{ }^{2} H \rightarrow J / \psi+\Delta^{++}+\Delta^{-}$where transverse momenta of $J / \psi$ and one of $\Delta$ 's are back to back. The advantage of this reaction as compared to medium energy processes is the absence of a non-vacuum exchange in t -channel.

## Slow neutrons and final-state interaction length

Kai Gallmeister, Ulrich Mosel

With collider kinematics, it is very instructive to look at "slow" nucleons of energy less than 10 GeV , considered slow with respect to the (fast) target nucleon [1071], see also Section [5.12. Performing some exploratory simulations within the GiBUU framework (see Section (5.10) we are confronted with a lot of complications. In Fig. 5.83 we show some distributions of slow neutrons as a function of energy for different production points in the longitudinal axis, normalized to the corresponding number of scattered electrons. This result is to be considered as preliminary, since we learned that we need a more accurate treatment of Pauli-blocking and binding effects in the few MeV region. In addition, we need to take into account the production of slow nucleons via evaporation and fragmentation. This work is currently in progress by inclusion of a multi-fragmentation framework (SMM) [1089] and correcting for effects of the large energy gap between initial interaction and fragmenting nucleons.

It has been proposed by Ciofi degli Atti and coworkers in many papers (see Section 5.12) that the interaction cross section of the jet particles within a SIDIS event with the debris of the target nucleus shows interesting formation length dependencies. We see a large potential for our GiBUU model to study all these questions.

### 5.13 Bose-Einstein correlations at an electron-ion collider

Gerald P. Gilfoyle

QCD directs the formation of hadrons from quarks and gluons in hard scattering. However, our understanding of this process is ad hoc; there is no full, QCD-based theory to explain hadronization and fragmentation. To probe these processes, we propose to take advantage of an iconic quantum mechanical effect, the symmetrization of the wave function required for bosons. Particles formed near one another will have overlapping wave functions and the interference of the wave functions produces correlations in the intensity and momentum dependence of the final particles. These Bose-Einstein Correlations (BEC) (or the Hanbury-Brown Twiss effect) are examples of intensity interferometry and can be used to study the space-time extent of the source of the particles and/or learn about the dynamics of their formation. They have been used to investigate hot nuclear matter, but there are only a few cases where $e+A$ interactions have been studied. That work revealed that BECs can be used to study the QCD string in hard scattering and our simulations show we will be able to make precise measurements of the BEC source size at an EIC.

Bose-Einstein Correlations arise when two identical bosons are detected and their joint wave function $\left|p_{1} p_{2}\right\rangle$ ( $p_{i}$ is the particle 4 -momentum) must be symmetric under particle exchange. In other words, when the two bosons are detected from different points in spacetime, the observer cannot distinguish the origin of each particle so their amplitudes must add. This requirement gives rise to interference terms in the intensity that do not exist for non-identical particles. In fact, for identical fermions there would an anti-correlation between the particles. The BEC in energy-momentum space is related to the extent of the source in its spatial dimensions and the correlation function can be written as

$$
\begin{equation*}
R\left(Q_{12}\right)=\frac{d N / d Q_{12}}{d N_{\text {ref }} / d Q_{12}} \tag{5.175}
\end{equation*}
$$

where $Q_{12}=\sqrt{-\left(p_{1}-p_{2}\right)^{2}}$ is the Lorentz-invariant momentum difference between the identical bosons and $N_{\text {ref }}$ is a reference spectrum constructed with no BECs. The correlation function is often parameterized as

$$
\begin{equation*}
R\left(Q_{12}\right)=\alpha\left(1+\lambda \Omega\left(Q_{12} r_{12}\right)\right)\left(1+\beta Q_{12}\right) . \tag{5.176}
\end{equation*}
$$

In static models of particle sources, $\Omega\left(Q_{12} r_{12}\right)$ can be interpreted as the Fourier transform of the spatial distribution of the emission region of bosons with overlapping wave functions and is characterized by the size parameter $r_{12}$ of the source. It is typically treated as a Gaussian $\left(e^{-Q_{12}^{2} r_{12}^{2}}\right)$ or an exponential $\left(e^{-Q_{12} r_{12}}\right)$. The parameter $\lambda$ measures the coherence of the source, $\alpha$ is a normalization factor, and $\beta$ accounts for long range correlations.
Existing measurements. There is a long history of the study of BECs in particle and nuclear physics going back to 1960 when two-pion correlations were measured in $p \bar{p}$ collisions [1091. They have been used to study geometric properties in $e+p$ reactions [1090], the space-time extent of hot nuclear matter in $A u+A u$ collisions [1092, 1093], and the dynamical properties of hadrons extracted from $A u+A u$ collisions [1094]. Figure 5.84 shows the two-pion correlation function from Ref. [1090] for $e+p$ reactions measured at the DESY collider for an electron momentum $p_{e}=27.6 \mathrm{GeV}$ and proton momenta $p_{p}=-820 \mathrm{GeV}$ and $p_{p}=-920 \mathrm{GeV}$. It shows several of the important features seen in many correlation functions. There is a clear correlation that is maximal at $Q_{12}=0$ and drops rapidly to unity


Figure 5.84. Left: the measured Bose-Einstein correlation function, $R\left(Q_{12}\right)$, together with Gaussian and exponential fits 1090. The error bars show the statistical uncertainties. The data points included in the fit are marked with the circles. The other points are excluded from the fit because the correlation is dominated by resonance effects. Right: Pythia simulation of $\pi^{+} \pi^{+}$Bose-Einstein correlations (BEC) at Electron-Ion Collider kinematics. The BEC parameters were taken from Ref. [1090. The Lund fragmentation model was used.
and below with increasing momentum difference. The height of the correlation function at $Q_{12}=0$ measures the coherence in the source. At moderate $Q_{12}$ the correlation drops below one, reflecting the usual practice of requiring the integral of the entire correlation function to go to one. There is a steady rise in $R$ at larger $Q_{12}$ due to long-range effects. Recall the denominator Eq. (5.175); It should be free of the correlations arising from Bose-Einstein statistics, but will not be free of all correlations: momentum conservation will push $R$ up at large $Q_{12}$. The width of the peak at $Q_{12}=0$ reflects the size of the source of the two bosons, i.e. large width in momentum space implies a small spatial source. The width of $R$ in Fig. 5.84 corresponds to $r_{12} \approx 0.9 \mathrm{fm}$ for an exponential fit and is largely independent of $Q^{2}$, the square of the four-momentum transfer.
BECs at an EIC. Measurements with the CLAS detector of a different type of correlations (i.e., two protons) have been performed on nuclear targets. Some of the results are shown in the left-hand panel of Fig. 5.85 (1095). The figure shows the effects on the source size $r_{r m s}$ (extracted from the correlation) of the average pair momentum $\left(p=\left|\vec{p}_{1}+\vec{p}_{2}\right| / 2\right)$ and the nuclear size on the correlation function. At low average pair momentum $r_{r m s}$ increases for the heavier nuclei and approaches the nuclear size; implying the possible dominance of proton rescattering. The density of the source was extracted in Ref. [1095] and found to be about 2-3 times the nuclear density in helium. In the right-hand panel of Fig. 5.85 we show preliminary results on $\pi^{+} \pi^{+}$pairs on several nuclear targets [1099]. Below $Q_{12} \approx$ $0.15 \mathrm{GeV} / \mathrm{c}$ the correlations from all nuclei rise to a large positive correlation. Above $Q_{12} \approx 0.15 \mathrm{GeV} / \mathrm{c}$ the correlation functions overlap one another within the statistical uncertainty.

Measurement of Bose-Einstein correlations at an EIC will provide a new portal to studies of cold, high-density nuclear matter and the process of hadronization. The ground-state properties of nuclei are now well understood. Ab initio calculations of the nuclear ground state are successful for nuclei up to $A=8$ and higher [1100, 1101] and lattice QCD calculations continue to make progress toward a fundamental understanding of the nucleon


Figure 5.85. Left panel: The size parameter $r_{r m s}$ as a function of the mean pair momentum $p=$ $\left|\vec{p}_{1}+\vec{p}_{2}\right| / 2$ is shown for different nuclear targets [1095]. Data from Refs [1096, 1097, 1098, are shown which correspond to $e-{ }^{16} \mathrm{O}$ interactions at initial energy of 5 GeV and $Q^{2}<0.1(\mathrm{GeV} / \mathrm{c})^{2}$ are shown for comparison. Right panel: Preliminary correlation functions for $\pi^{+} \pi^{+}$from the CLAS detector at Jefferson Lab [1099.
[1102]. However, the high-momentum components of the nuclear ground state are only now being revealed. These high-momentum nucleons are often paired with another, nearby neutron or proton forming regions of cold, dense nuclear matter. Short-range correlations have shown the importance of high-density components and the influence of the tensor force [1103, 1104]. The results of Ref. [1095] (left-hand panel of Fig. 5.85) demonstrated the use of correlations to extract density information. Measurements at an EIC could also help us to understand neutron stars [1105] and the EMC effect [1106].
Simulations. We have simulated Bose-Einstein correlations for $\pi^{+} \pi^{+}$pairs at the kinematics of an Electron-Ion Collider to investigate the feasibility of measuring BECs at an EIC. For our starting point we used the results for $\pi^{+} \pi^{+}$correlations from ep reactions at DESY that are shown in Fig. 5.84 [1090]. That measurement covered the range $Q^{2}=4-8000(\mathrm{GeV} / \mathrm{c})^{2}$ and there was limited $Q^{2}$ dependence in the BEC parameters they extracted. It is reasonable to believe those parameters may also apply to the EIC kinematics. We chose the $\pi^{+} \pi^{+}$ channel because we expect them to be abundant and there is data from other experiments that enable us to make comparisons. We took advantage of several existing tools to perform the simulations. The Pythia program [81] was used to generate events with either Lund string model or independent fragmentation. The code also includes a feature to simulate Bose-Einstein correlations [1107, 1108]. The algorithm for the BECs starts with the usual fragmentation simulation and then pairs of identical particles (i.e. $\left.\pi^{+} \pi^{+}\right)$are selected. For these pairs the relative 4-momentum $Q_{12}$ is modified according to the desired parameterization (see discussion of Eq. (5.176) above) with the constraint that the total 3-momentum of the pair remains the same in the center-of-mass (CM). The overall effect of applying the algorithm is to preserve momentum conservation, but reduce the energy. To compensate for the energy reduction, the CM momentum vectors are then rescaled.

As a consistency check, we compared the simulated correlation function $R$ for $\pi^{+} \pi^{+}$ pairs with the measurements from DESY shown in Fig. 5.84. The simulated correlation was weaker than the measured one, $R\left(Q_{12}=0\right)=1.2$ (simulated) versus $R\left(Q_{12}=0\right)=1.38$ (measured), and not as wide, but still experimentally significant. Since we are studying the possibility of observing BECs, the parameters from Ref. 1090 will provide a more


Figure 5.86. Longitudinal and transverse ( $L T$ ) correlation functions calculated with Pythia. The left-hand panel shows the correlations functions using the Ref. 1090 parameters. The other two panels show a comparison between those results and ones from a calculation with a smaller source size $r_{12}$.
conservative (and safer) test. We also simulated the BECs at the same kinematics as the preliminary results shown in the right-hand panel of Fig. 5.85 ( $p_{e}=5 \mathrm{GeV}$ and fixed target). Here we found the simulated correlation disappeared entirely. The multiplicity of the events generated by Pythia dropped significantly at these kinematics reflecting the limitations of the code at these lower energies.

At EIC kinematics ( $p_{e}=11 \mathrm{GeV} / \mathrm{c}$, $p_{i o n}=-60 \mathrm{GeV} / \mathrm{c}, \sqrt{s}=51 \mathrm{GeV}$ ), we used the BEC parameters from ZEUS [1090]. Since the EIC will run at energies lower than at HERA, but above the current ones at Jefferson Lab, our estimates of the BECs are again conservative ones. Our simulation of $R$ at EIC kinematics is shown in the right panel of Fig. [5.84. There is, like in the Ref. [1090] data, a sizable correlation at $Q_{12}=0$, a decrease in $R$ with width $\approx 0.2 \mathrm{GeV} / \mathrm{c}$, a dip below unity (recall discussion of Fig. 5.84) and then the data approach one at high $Q_{12}$. The Lund model was used here for the fragmentation and a calculation using the independent fragmentation model in Pythia yielded similar results. This result shows we can expect sizable correlation functions at the EIC.

One of the possible effects we may see at an EIC is the stretching of the QCD color string at high $Q^{2}$ and/or changes in the string tension (recall Ref. [1109]). The fragmentation region may not be spherical as observed in Ref. [1109, but may have different sizes in the longitudinal and transverse directions. Such a difference was measured in Ref. 1090 where the longitudinal radius was $0.26 \pm 0.03 \mathrm{fm}$ bigger than the transverse one. To search for such an effect in our simulation requires a different approach to extracting $R$. We worked in the longitudinal Center-of-Mass System (LCMS), where the longitudinal components of the pair momentum add to zero and extracted the transverse and longitudinal 3-momentum differences $\Delta p$. Our initial results are shown in the left-hand panel of Fig. 5.86. The transverse (red, filled circles) and longitudinal (blue, open circles) produce the characteristic shapes seen above for $R$, but with significant quantitative differences between the two. The transverse correlation is about twice the longitudinal one at $Q_{12}=0$ and the widths are similar. The large difference between the correlation functions suggests this may be a useful tool for studying space-time properties of the emission source. To delve deeper into this question, we considered the sensitivity of the $L T$ distributions to changes in the size parameter in the BEC parameterization. The middle and right-hand panels in Fig. 5.86 show a comparison of the same $L T$ correlation functions shown in the left-hand panel with ones calculated with a smaller size parameter $\left(r_{12}=0.73 \mathrm{fm}\right.$ versus $r_{12}=0.93 \mathrm{fm}$
from Ref. [1090). The smaller radius amplifies the shape of the correlation functions (the maximum at $Q_{12}=0$ increases and the dip at $Q_{12} \approx 0.6 \mathrm{GeV} / \mathrm{c}$ is deeper. We can clearly separate the two distributions within the Monte Carlo statistics shown here. We expect the statistical uncertainties for an EIC measurement to be better than the Monte Carlo statistical uncertainties shown here. The cross sections for these reactions (from Pythia) multiplied by the EIC luminosity suggest a production rate of $10^{5} \mathrm{~Hz}$. We also fitted the correlation functions with Eq. (5.176) and obtained uncertainties on the size parameter $r_{12}$ less than 0.15 fm which is comparable to the precision of the results in Ref. [1090]. Thus, we will be able to discriminate between different size parameters at least at the 0.2 fm level. Conclusions. Bose-Einstein correlations will be an important tool at an Electron-Ion Collider for studying high-density nuclear matter, the dynamics of the QCD string in hard scattering, and to gain a deeper understanding of fragmentation and hadronization. Our simulations have shown us that we can expect large (20\%) effects in the correlation function at small $Q_{12}$. The longitudinal-transverse correlations are sensitive to the size parameter to a fraction of a fm . Finally, the large $\pi^{+} \pi^{+}$BECs observed at JLab that are not reproduced in our simulations hold the promise of new physics to be uncovered with the EIC.

## $5.14 \mathrm{e}+\mathrm{A}$ Monte Carlo simulation tools

### 5.14.1 A Monte Carlo Generator for Diffractive Events in e+A Collisions

Tobias Toll and Thomas Ullrich

While there is a rich set of Monte Carlo (MC) event generators for $e+p$ collisions available (e.g. PYTHIA6 [110], HERWIG++ [1111, LEPTO [91], PEPSI [155], RAPGAP [1112], ARIADNE [1113], CASCADE [1114, SHERPA [1115]), the situation for eA collisions is less favorable. The exception is DPMJET [1116 which attempts to describe deep-inelastic $e \mathrm{~A}$ events but does not include the rich physics accessible via diffractive events.

In strong interactions, diffractive events can be interpreted as resulting from scattering via the exchange of a pomeron that carries the quantum numbers of the vacuum, as discussed in 5.4. It was a surprise to see that a large fraction (approximately $15 \%$ ) of all $e+p$ events at HERA were diffractive. Calculations predict this fraction to be even larger in $e+\mathrm{A}$ collisions at EIC where the large nuclei remain intact $\sim 25-30 \%$ of the time (e.g. [826, 825]). In fact diffractive events are considered the most sensitive means of studying saturation since the dipole scattering amplitude is proportional to the square of the gluon momentum distribution $x g\left(x, Q^{2}\right)$. Another fascinating aspect of the study of diffractive events at an EIC is that that it would allow us to measure the intensity and the spatial distribution of the strong field that binds the nucleus together [885].

For all the above measurements the most important process to study is the production of exclusive diffractive vector mesons, such as $J / \Psi, \phi$, and $\rho$ mesons, as well as Deeply Virtual Compton Scattering (DVCS) photons. These processes give very clean final states, consisting of the scattered electron and nucleus and one extra particle: a vector meson or a real photon. This is a process which is dominated by small momentum fractions $x<10^{-2}$. $J / \Psi$ production is particularly well suited for studies of the spatial gluon distribution inside nuclei due to its well known wave function, narrow decay width, and its large branching ratio for electromagnetic decays $J / \Psi \rightarrow e^{+}+e^{-}\left(\right.$or $\left.\mu^{+}+\mu^{-}\right)$.

The measurement of exclusive vector meson production in diffractive events will be one of the key measurements at an EIC. Therefore these processes has been the starting point in our efforts to realise a new multi-purpose MC generator.
The Dipole Model: The dipole model is an important tool in investigations of diffractive processes and for the purpose of applying it to $e+$ A collisions, we needed an impact parameter dependent model as starting-point. Two known models fulfil this requirement: bSat (or IPSat) 823] and bCGC [823, 824]. They are the underlying building blocks used in the generator. In what follows, we will concentrate on the bSat model and not discuss the technical details of the generator but focus on how the dipole models are applied with emphasis on the extension to $e+$ A collisions.

The parameters of the dipole models described below have been tuned to inclusive HERA data, and they describe a wide variety of HERA measurements exceptionally well [823, 824].

The Dipole Model in $e+p$ : The production of exclusive vector mesons and DVCS photons at small $x$ for ep collisions, $e+p \rightarrow e^{\prime}+p^{\prime}+V / \gamma$, in the dipole model has been extensively studied [823, 824]. Here the virtual photon splits into a quark-antiquark dipole which interacts with the target diffractively via one or many two-gluon pomeron exchanges


Figure 5.87. (a) shows the dipole cross-section for various impact parameters as a function of dipole size in the bSat model. (b) and (c) depict the wave overlap functions for $J / \Psi$ and $\rho$ mesons respectively as a function of $r$ for various $Q^{2}$ for transversely polarized photons (from [823]).
(see Fig. 3.14). The amplitude for this process is

$$
\begin{equation*}
\mathcal{A}_{T, L}^{\gamma^{*} p \rightarrow V p}(x, Q, \boldsymbol{\Delta})=i \int \mathrm{~d}^{2} \mathbf{r} \int \frac{\mathrm{~d} z}{4 \pi} \int \mathrm{~d}^{2} \mathbf{b}\left(\Psi_{V}^{*} \Psi\right)(r, z) e^{-i \mathbf{b} \cdot \boldsymbol{\Delta}} \frac{\mathrm{~d} \sigma_{q \bar{q}}^{(p)}}{\mathrm{d}^{2} \mathbf{b}}(x, r, \mathbf{b}) \tag{5.177}
\end{equation*}
$$

Here $T$ and $L$ represent the transverse and longitudinal polarizations of the virtual photon, $r$ is the size of the dipole, $z$ the energy fraction of the photon taken by the quark, $\Delta=\sqrt{-t}$ is the transverse part of the four-momentum difference of the outgoing and incoming proton, and $\mathbf{b}$ is the impact parameter of the dipole. The wave function of the produced vector meson or real photon is $\Psi_{V}$ while that of the incoming photon that splits into the dipole is $\Psi$.

In the bSat model the dipole cross-section in terms of the dipole scattering amplitude $\mathcal{N}^{(p)}(x, r, \mathbf{b})$ is

$$
\begin{equation*}
\frac{\mathrm{d} \sigma_{q \overline{\mathrm{q}}}^{(p)}}{\mathrm{d}^{2} \mathbf{b}} \equiv 2 \mathcal{N}^{(p)}(x, r, \mathbf{b})=2\left[1-\exp \left(-\frac{\pi^{2}}{2 N_{C}} r^{2} \alpha_{S}\left(\mu^{2}\right) x g\left(x, \mu^{2}\right) T(b)\right)\right] \tag{5.178}
\end{equation*}
$$

where $\mu^{2}=4 / r^{2}+\mu_{0}^{2}$ and $\mu_{0}^{2}$ is a cut-off scale in the DGLAP evolution of the gluons $g\left(x, \mu^{2}\right)$. The nucleon shape function $T^{(p)}(b)=1 /\left(2 \pi B_{G}\right) \exp \left(-b^{2} /\left(2 B_{G}\right)\right)$. The parameter $B_{G}$ is determined through fits to HERA data 823 ]. We use $B_{G}=4 \mathrm{GeV}^{-2}$. It should be noted that bSat is a model of multiple two-gluon exchanges and does not contain any gluon-gluon recombinations. It is however, by construction, a model that obeys unitarity, so in this respect it is a saturation model.

Figure 5.87(a) shows the dipole cross-section as a function of $r$ for different impact parameters. Figure 5.87(b) and (c) depict the wave overlap, $\left(\Psi_{V}^{*} \Psi\right)(r, z)$, for $J / \Psi(\mathrm{b})$ and $\rho$ mesons (c) 823] used in Eq. 5.177. It should be noted that the $J / \psi$ is not necessarily the best suited vector meson for probing saturation effects. Studying saturation implies probing large dipole radii $r \gtrsim 2 \mathrm{GeV}^{-1}(0.4 \mathrm{fm})$. However, the wave overlap with the $J / \Psi$ vanishes almost entirely for these dipole sizes. The lighter vector mesons $\rho$ and $\phi$ certainly appear more suited in this case. Unfortunately the wave functions of the lighter vector mesons are less well known than that of the $J / \Psi$ increasing the uncertainties in model-data
comparisons. This can be overcome in the future by improving our knowledge of the light vector meson wave functions.
Phenomenological Corrections to the Cross-Section: In the derivation of the dipole amplitude (eq. (5.177)) only the real part of the $S$-matrix is taken into account, making the amplitude purely imaginary. The real part of the amplitude can be included by multiplying the cross-section by a factor $\left(1+\beta^{2}\right)$, where $\beta$ is the ratio of real to imaginary part of the amplitude. It is calculated using

$$
\begin{equation*}
\beta=\tan \left(\lambda \frac{\pi}{2}\right), \quad \text { where } \lambda \equiv \frac{\partial \ln \left(\mathcal{A}_{T, L}^{\gamma * p \rightarrow V p}(x, Q, \Delta)\right)}{\partial \ln (1 / x)} \tag{5.179}
\end{equation*}
$$

Also, the two gluons interacting in each event do not carry the same momentum fraction $x$. In the leading $\ln (1 / x)$ limit, this skewedness effect disappears, but can still be accounted for by a factor $R_{g}(\lambda)$, where $R_{g}(\lambda)=2^{2 \lambda+3} \Gamma(\lambda+5 / 2) / \Gamma(\lambda+4) / \sqrt{\pi}$.
$R_{g}$ is multiplied to the gluon distribution $x g\left(x, \mu^{2}\right)$ and $\lambda$ is defined as the derivative of $\ln \left(x g\left(x, \mu^{2}\right)\right)$ with respect to $\ln (1 / x)$. It should be noted that while the correction of the real part of the amplitude is on firm theoretical footing, the skewedness correction should be viewed as a purely phenomenological correction. Also, the correction variable $\lambda$ is only well behaving for small values of $x<10^{-2}$. The combined magnitude of both corrections is $x$ dependent and is typically of the order of $10-60 \%$.

Extending the Dipole Model from $e+p$ to $e+A$ : When going from $+e p$ to $e+\mathrm{A}$ scattering we will use the independent scattering approximation (see also eq. (5.95)),

$$
\begin{equation*}
1-\mathcal{N}^{(A)}=\prod_{i=1}^{A}\left(1-\mathcal{N}^{(p)}\left(x, r,\left|\mathbf{b}-\mathbf{b}_{i}\right|\right)\right) \tag{5.180}
\end{equation*}
$$

where $\mathbf{b}_{i}$ is the position of each nucleon in the nucleus. Here, these positions are generated according to the Wood-Saxon potential. Combining equations (5.178) and (5.180) the bSat dipole cross-section for $e+\mathrm{A}$ becomes:

$$
\begin{equation*}
\frac{\mathrm{d} \sigma_{q \bar{q}}^{(A)}}{\mathrm{d}^{2} \mathbf{b}}(x, r, \mathbf{b}, \Omega)=2\left[1-\exp \left(-\frac{\pi^{2}}{2 N_{C}} r^{2} \alpha_{S}\left(\mu^{2}\right) x g\left(x, \mu^{2}\right) \sum_{i=1}^{A} T^{(p)}\left(\mathbf{b}-\mathbf{b}_{i}\right)\right)\right] \tag{5.181}
\end{equation*}
$$

At small gluon momentum fractions, $x<10^{-2}$, the dipole interacts coherently with large volumes of the nucleus. Therefore the configuration of nucleons in the nucleus is not an observable. To obtain the total cross-section, these nucleon configurations have to be averaged over:

$$
\begin{equation*}
\left.\frac{\mathrm{d} \sigma_{\text {total }}}{\mathrm{d} t}=\left.\frac{1}{16 \pi}\langle | \mathcal{A}\left(x, Q^{2}, t, \Omega\right)\right|^{2}\right\rangle_{\Omega} \tag{5.182}
\end{equation*}
$$

where $\Omega$ denotes nucleon configurations.
One defines two different kinds of diffractive events in $e A$ : coherent and incoherent. In incoherent diffractive processes the nucleus breaks up into two or more color neutral fragments, something not possible in diffractive $e p$. If the nucleus stays intact the diffractive processes are coherent. In the Good-Walker picture [1117] (also found in [885]) the incoherent cross-section is proportional to the variance of the amplitude with respect to the initial nucleon configurations $\Omega$ of the nucleus:

$$
\begin{equation*}
\left.\frac{\mathrm{d} \sigma_{\text {incoherent }}}{\mathrm{d} t}=\frac{1}{16 \pi}\left(\left.\langle | \mathcal{A}\left(x, Q^{2}, t, \Omega\right)\right|^{2}\right\rangle_{\Omega}-\left|\left\langle\mathcal{A}\left(x, Q^{2}, t, \Omega\right)\right\rangle_{\Omega}\right|^{2}\right) \tag{5.183}
\end{equation*}
$$

where the first term on the R.H.S is the total cross-section and the second term is the coherent part of the cross-section.
The Generator: The Monte Carlo event generator is implemented in C++ through a set of modular classes. A rich set of input parameters let the user select beam energy and species (A), wave function model, dipole model, kinematic range and the final state particle to study: $\rho, \pi, J / \Psi$, or $\gamma$ (DVCS). Internally, the variables $t, Q^{2}$, and $W^{2}$ are generated following a probability density function (pdf). From these three variables, the complete final state consisting of the scattered electron, the scattered proton or nucleus, and the produced vector meson or photon can be unambiguously calculated.

Generating Events for ep: The variables are generated from a probability density function which for $e p$ is

$$
\begin{equation*}
\operatorname{pdf}\left(Q^{2}, W^{2}, t\right)=\frac{\partial^{3} \sigma_{\mathrm{tot}}}{\partial Q^{2} \partial W^{2} \partial t}=\frac{1}{16 \pi} \sum_{T, L} f_{T, L}^{\gamma^{*}}\left(Q^{2}, W^{2}\right)\left|\mathcal{A}_{T, L}^{\gamma^{*} p \rightarrow V p}\left(W^{2}, Q^{2}, t\right)\right|^{2} \tag{5.184}
\end{equation*}
$$

where $f_{T, L}^{\gamma^{*}}$ is the photon flux for transversely and longitudinally polarized photons. The user may also choose to include the corrections for the real part of the amplitude and/or the skewedness effect as described above.
Generating Events for $e \mathbf{A}$, the MC-Glauber Approach: For $e \mathrm{~A}$ the pdf is

$$
\begin{equation*}
\left.\frac{\partial^{3} \sigma_{\text {total }}}{\partial Q^{2} \partial W^{2} \partial t}\left(Q^{2}, W^{2}, t\right)=\left.\frac{1}{16 \pi} \sum_{T, L} f_{T, L}^{\gamma^{*}}\left(Q^{2}, W^{2}\right)\langle | \mathcal{A}_{T, L}^{\gamma^{*} A \rightarrow V A}\left(Q^{2}, W^{2}, t, \Omega\right)\right|^{2}\right\rangle_{\Omega} \tag{5.185}
\end{equation*}
$$

Here the average of an observable $\mathcal{O}$ with respect to the initial nucleon configurations $\Omega$ is defined as $\langle\mathcal{O}\rangle_{\Omega} \equiv \frac{1}{C_{\max }} \sum_{j=1}^{C_{\text {max }}} \mathcal{O}\left(\Omega_{j}\right)$, where a number of $C_{\text {max }}$ configurations $\Omega_{j}$ are generated and summed over. This sum will converge to the true average for large $C_{\max }$. We call this way of performing the average the MC-Glauber approach. It should be noticed that this method of averaging the initial nucleon configurations is different than in previous publications, e.g. in 826] and 885].

For each event, the coherent part of the cross-section is calculated simultaneously with the total cross-section, by averaging the amplitude before squaring it. It is then decided probabilistically that the nucleus breaks up if

$$
\begin{equation*}
\left(\frac{\partial^{3} \sigma_{\text {total }}}{\partial Q^{2} \partial W^{2} \partial t}-\frac{\partial^{3} \sigma_{\text {coherent }}}{\partial Q^{2} \partial W^{2} \partial t}\right) / \frac{\partial^{3} \sigma_{\text {total }}}{\partial Q^{2} \partial W^{2} \partial t}>R \tag{5.186}
\end{equation*}
$$

where $R$ is a random number from a uniform distribution on $[0-1]$. When this happens, the final state does not contain a scattered nucleus but rather the decay products resulting from the break-up of the nucleus.
Generating Events for $e \mathbf{A}$, the Optical Approach: A simpler and faster way of doing the average over the initial nucleon configurations is what we call the optical approach. Here the average is done implicitly in the dipole cross-section which becomes 826

$$
\begin{equation*}
\left\langle\frac{\mathrm{d} \sigma_{q \bar{q}}^{A}}{\mathrm{~d}^{2} \mathbf{b}}\right\rangle_{\Omega, \text { Optical }}=2\left[1-\left(1-\frac{T_{A}(\mathbf{b})}{2} \sigma_{q \bar{q}}(x, r)\right)^{A}\right] \tag{5.187}
\end{equation*}
$$

For processing speed reasons we approximate the integrated dipole cross-section using the GBW model 819]:

$$
\begin{equation*}
\sigma_{q \bar{q}}^{\mathrm{GBW}}(x, r)=\sigma_{0}\left(1-\exp \left(-\frac{r^{2} Q_{s}^{2}(x)}{4}\right)\right) \tag{5.188}
\end{equation*}
$$



Figure 5.88. Left plot. The coherent part of the cross-section as a function of $|t|$ for electron-gold scattering at $Q^{2}=10^{-4} \mathrm{GeV}^{2}$ and $x_{p}=0.006$ averaged over $40,80,160$ and 500 configurations respectively. Right plot. The total, coherent, and incoherent cross-sections as a function of $|t|$ for $e \mathrm{Au}$ scattering at $Q^{2}=10^{-4} \mathrm{GeV}^{2}$ and $x_{p}=0.006$ averaged over 500 configurations.
where $Q_{s}^{2}(x)=\left(x_{0} / x\right)^{\lambda}$. Here, $\sigma_{0}=23.9 \mathrm{mb}, \lambda=0.287$ and $x_{0}=1.1 \cdot 10^{-4}$ [823]. $T_{A}$ is the projection of the Woods-Saxon potential in the transverse plane. This approximation is valid for large nuclei. In the optical approach, only the coherent part of the cross-section can be calculated, since it gives the average of the amplitude, but not of the amplitude squared. It is implemented in the program as a fast alternative to the more accurate but CPU-time intensive MC-Glauber approach.
Results: In the following we only show results from the $e+\mathrm{A}$ part of the generator. In Figure 5.88, the coherent part of the crosssection for $e+\mathrm{A} \Rightarrow e^{\prime}+\mathrm{A}^{\prime}+J / \Psi$ is shown as a function of $|t|$, with $Q^{2}=10^{-4} \mathrm{GeV}^{2}$ and $x_{p}=0.006$. The nucleus used is gold with $\mathrm{A}=197$. The cross-section is calculated for different numbers of averaged nucleon configurations $C_{\text {max }}$. The target is probed by the dipole at a scale $\Delta$ which means that at large $|t|$ the cross-section is much more sensitive to smaller variations in the positions of the nucleons than it is for small $|t|$. Therefore, for small $|t|$, the sum over configurations converges quickly, while for larger $|t|$, more configurations are needed for the sum to converge. As indicated in Fig. 5.88 approximately 100 configurations are needed to describe $e \mathrm{~A}$ scatterings up to $|t| \approx 0.2 \mathrm{GeV}^{2}$. In Figure 5.88 the total


Figure 5.89. The coherent part of the cross-section of $e+\mathrm{A} \rightarrow e^{\prime}+\mathrm{A}^{\prime}+J / \Psi$ for two different distributions of the initial nucleon configurations: WoodsSaxon and KLN (from [1118]). cross-section and the incoherent part of the cross-section are shown as averaged over 500 nuclear configurations. The $t$-slope of the incoherent cross-section is close to $6 \mathrm{GeV}^{-2}$. This is a bit steeper than is found in [827, where the impact parameter dependence was factorized out in the dipole cross-section and therefore the $t$-slope $=B_{G}=4 \mathrm{GeV}^{-2}$.

In order to measure the spatial distribution of gluons inside the nucleus, the coherent cross-section has to be well measured as a function of $t$. The inverse Fourier transformation
of this will then give the transverse spatial dependence of the amplitude. To do this the position of the several coherent maxima in the $t$-distribution have to be measured accurately.

Experimentally, this requires the suppression of the large incoherent fraction, which is of course also of great interest in itself [825]. Coherent and incoherent processes can be separated by detecting the nuclear-breakup, i.e., detecting the nuclear fragments. While this is experimentally straight forward in fixed target experiments it is rather challenging at an EIC since the charged fragments are transported along the ion beam line. The most promising approach is the measurement of emitted neutrons via zero-degree-calorimeters, a technique used extensively at RHIC. Preliminary studies using de-excitation models (e.g. Gemini $++[1119$ and SMM [1120]) and a realistic layout of an EIC interaction region showed that rejection factors of larger than $10^{5}$ can be achieved.

In Fig. 5.88, the nucleon configurations have been explicitly generated according to the Woods-Saxon configuration. Fig. 5.89 shows the same Woods-Saxon distribution in the optical approach compared with a KLN distribution motivated by the CGC as discussed in [1118]. It can be seen that the difference when using different initial nucleon distributions within the nucleus is considerable and easily measurable by an EIC. It also demonstrates the flexibility of the generator in adapting different models at all stages of the generation process.
Summary and Outlook: A new event generator for the generation of diffractive events in $e p$ and $e \mathrm{~A}$ collisions has been implemented based on an impact parameter dependent dipole model. It describes the coherent and incoherent contributions to the cross-sections. In its current version it is limited to the production of exclusive vector mesons and DVCS photons. We intend to include more general diffractive processes in the same framework, $e+p / \mathrm{A} \rightarrow e^{\prime}+p^{\prime} / \mathrm{A}^{\prime}+X$ where $X$ is a general final state consisting of two or more hadrons. When completed it will be the first diffractive event generator for $e \mathrm{~A}$ collisions with a broad range of processes relevant for the physics of a future EIC.

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### 5.14.2 Parton propagation and hadronization simulations: overview

## Alberto Accardi

The "Parton Propagation and Fragmentation" working group is currently working on several Monte Carlo simulations to address hadronization in the cold nuclear medium. More information, references and links are available on the PPF working group wiki [1121].

- PyQM. The "Pythia Quenching Model" is an energy-loss simulation based on Pythia, see Section 5.14.3. The partons created in the hard scattering are allowed to lose energy according to the Salgado-Wiedemann quenching weights, and then fed into the Lund string fragmentation Pythia module. The goal is to determine if the Lund string fragmentation leads to observable differences compared to using Fragmentation Functions to describe leading hadron attenuation (as implemented e.g. in PQM, see below), and to provide a simulation for a broader range of hadron flavors.
- Q-Pythia extension to DIS. Q-Pythia is an energy loss simulation by Armesto, Cunqueiro and Salgado based on medium-modified DGLAP evolution equations. Cur-
rently, only energy loss in the QGP is implemented, and we are working on implementing energy loss in the cold nuclear target. Pursuing this simulation is likely to have a very big pay-off: it will allow to study jet nuclear modifications, the effects of medium modified DGLAP evolution on hadron observables, and compare this to the BDMPS energy loss formalism in the integrated PQM simulation, and the implementation of the Higher-Twist energy loss formalism. Comparison to simulations done with Q-Herwig, would also allow one to gauge the effects of cluster vs. Lund string hadronization.
- PQM. The "Parton Quenching Model" is a simulation by Dainese, Loizides and Paic, which uses Pythia as a parton level generator, and then applies the SalgadoWiedemann quenching weights to determine the parton energy loss before using Fragmentation Functions to determine single hadron attenuation. It has been integrated in Q-Pythia by C. Loizides.
- PyQM integration. It will be interesting to integrate PyQM in Q-Pythia, to provide a direct comparison between hadronization performed according to the Lund string model and using Fragmentation Functions.
- Higher-Twist energy loss. The Higher-Twist energy loss formalism has recently been extended to include a resummation of all higher-twist contributions, and inmplemented in a Monte-Carlo simulation, see Section 5.11,
- GiBUU. This is (among other things) a simulation of nuclear modifications of hadron production in DIS based on the Lund string model and BUU coupled-channel transport equation for the (pre)hadrons, and completely neglects energy loss, see Section 5.10. It has been extensively tested on HERMES and EMC data, and is ready to use at the EIC energy. It will be interesting to implement the few variations in the space-time prehadron production schemes available on the market and investigate possible observable differences. Inclusion of target fragmentation is currently in progress in the multi-fragmentation framework (SMM) 1089 and correcting for effects of the large energy gap between initial interaction and fragmenting nucleons.


### 5.14.3 PyQM: a pure energy loss Monte-Carlo simulation

## Raphaël Dupré and Alberto Accardi

Pure quark energy loss models are widely used to describe jet quenching in relativistic heavy ion collisions (RHIC), however most of the calculations were never applied to the nDIS experiments, which are usually at lower energy, making any comparison difficult. EIC is the chance to have data of both processes at similar kinematic, in this context it is natural to develop PyQM, a pure energy-loss Monte-Carlo simulation for nDIS based on the Salgado-Wiedemann quenching weights formalism [1122] widely used to analyze RHIC data. This simulation will be utilized as a tool to evaluate the future EIC capabilities concerning quark energy loss measurement; since it also provides rate estimates and the kinematics of particles to detect, this information will be used to discuss the relevance and interest of various observables and the accelerator and detector requirements to access them.

The PyQM Monte-Carlo simulation is based on PYTHIA [81] for the DIS interaction and the fragmentation process, which is described by the Lund string model. Between the intial hard scattering and string fragmentation, we apply quark energy loss on the struck
parton, using a nuclear density profile [1123] to estimate the quantity of matter the quark has to go through, and the Salgado-Wiedmann quenching weights [1124] to calculate the energy loss itself. To account for the geometry of the nuclei, we follow Ref. [1125], and pick randomly the interaction point according to the nuclear density distribution; the thickness of the nuclear matter seen by the parton is then given by $R=\frac{2 \bar{\omega}_{C}^{2}(\vec{b}, y)}{\int_{y}^{\infty} d z \hat{q}_{A}(\vec{b}, z)}$ with $y$ the position along the propagation direction with its origin at the interaction point, and $\vec{b}$ the transverse position of the y axis relative to the center of the nucleus. The characteristic energy $\omega_{C}$, and the local transport coefficient $\hat{q}$ are given by

$$
\begin{equation*}
\omega_{C}(\vec{b}, y)=\int_{y}^{\infty} d z(z-y) \hat{q}_{A}(\vec{b}, z) \quad \hat{q}_{A}(\vec{b}, y)=\frac{\hat{q}_{0}}{\rho_{0}} \rho_{A}(\vec{b}, y) \tag{5.189}
\end{equation*}
$$

Then the only free parameter for the quenching weights, and indeed for the whole simulation, is $\hat{q}_{0}$, the transport coefficient at the center of the nucleus. This is found to be $\hat{q}_{0}=0.6 \mathrm{GeV}^{2}$ $\mathrm{fm}^{-1}$ from a fit of the HERMES data [1029] (figure 5.90), in agreement with the analytic calculations of [1125, 1010]. A full description of the results of this simulation compared to HERMES would be beyond the scope of this presentation; here we note that its results are satisfactory for the multiplicity ratio, but require a seemingly too large $\hat{q}$ compared to HERMES data on pion $p_{T}$-broadening. We are currently working on an implementation of $p_{T}$-broadening in our simulation, which, puzzingly, appears instead to produce the right amount of integrated $p_{T}$ broadening as a function of $A$. This issue is directly linked to the quenching weight calculation and work is in progress to better understand it.


Figure 5.90. Multiplicity ratio of positive pions from HERMES [1029 (points) compared to the PyQM pure energy loss simulation (lines).

### 5.15 Connections to other fields

### 5.15.1 Gluon Tomography in Nuclei - The Heavy Ion Collision Initial State

William A. Horowitz

The main purpose of colliding large nuclei is the creation and study of the quark-gluon plasma (QGP), the deconfined state of QCD matter at high temperatures ( $T \sim 200 \mathrm{MeV}$ ) and low baryon chemical potential $(\mu \sim 0)$. Measuring the properties of the QGP is interesting as it is a known phase of the strong force, one of the four known forces in Nature. The QGP is fascinating from a theoretical standpoint as there exists the possibility of experimentally measuring the emergent many-body properties of the non-linear, nonAbelian QCD field theory. It was hoped that the collision of large, ultra-relativistic nuclei in a heavy-ion collision (HIC) might provide an experimental window with which to observe the properties of the QGP, and it appears that just such a novel phase of matter has been created at RHIC [1126, 1127, 1128, 1129, 1130].

But what are the properties of this QGP that has been created? Qualitatively: is the medium strongly or weakly coupled; what are its relevant degrees of freedom; does viscous relativistic hydrodynamics describe the bulk physics of the QGP; does either pQCD or the phenomenological string theory methods of the AdS/CFT correspondence or neither describe the physics of either the bulk medium or the high momentum probes of the medium? Quantitatively: what is the viscosity of the medium; what are the values of its transport coefficients? Is the QGP at RHIC the most perfect fluid created by mankind? The difficulty faced when trying to answer these questions is that a heavy-ion collision is an incredibly complex event. It is useful to think about a HIC, as currently best understood, as a series of separate stages: 1) $t=-\infty$, the time before overlap, when the nuclei are boosted to 200 GeV per nucleon at RHIC; 2) $t=0$, the actual collision of the nuclei and creation of large chromodynamic fields; 3 ) $0 \lesssim t \lesssim 1 \mathrm{fm} / \mathrm{c}$, the initial large chromodynamic fields rapidly thermalize; 4) $1 \lesssim t \lesssim 3 \mathrm{fm} / \mathrm{c}$, evolution as a QGP; 5) $3 \lesssim t \lesssim 4 \mathrm{fm} / \mathrm{c}$, hadronization; 6) 4 $\mathrm{fm} / \mathrm{c} \lesssim t \rightarrow \infty$, evolution as a hadron gas. A cartoon of a typical central heavy ion collision is shown in figure 5.91.


Figure 5.91. Cartoon of the stages of a heavy ion collision. Timescales are approximate.
As one can see, the system is in the QGP phase for only a brief period of its entire spacetime evolution! These times are important to understand not only because they are interesting in their own right-What are the non-linear evolution effects on the color charge density of highly boosted nuclei? How do very large chromodynamic fields thermalize so rapidly? How does hadronization occur? -but also because the interpretation of experimental observables associated with the QGP is sensitive to the details of the physics of the other stages of a HIC. Any new means of experimentally extending our understanding of these other stages would provide a qualitative leap forward in our understanding of the


Figure 5.92. (a) Initial spatial anisotropy evolves into momentum anisotropy in non-central heavy ion collisions. Hydrodynamics aims to quantitatively model this process to gain information on the medium and its properties. (b) Comparison of data and theoretical predictions using viscous relativistic hydrodynamics for $v_{2}^{h}\left(N_{\text {part }}\right)$ (left) and $v_{2}^{h}\left(p_{T}\right)$ (right). Viscous hydrodynamics predictions use Glauber-like initial conditions (top) or a simplified implementation of color glass condensate (CGC) physics (bottom). Note the $100 \%$ difference in extracted $\eta / s$ from the two naive geometry models. figures adapted from [1131, 881].

QGP created at RHIC. Of particular importance are the initial conditions of a heavy-ion collision, from $t=-\infty$ to $t \sim 1 \mathrm{fm} / \mathrm{c}$, from the time before the collision up through thermalization. An electron-ion collider that probes gluons at $x \sim 10^{-3}$ could provide precisely this qualitatively new physics understanding of the initial conditions.

The two most striking discoveries of the RHIC heavy-ion program so far are perfect fluidity and jet suppression. The naive interpretation of the measured flow of low momentum particles is that the QGP is a strongly coupled fluid whose properties are described by AdS/CFT; the naive interpretation of the measured jet suppression is that the QGP is a weakly coupled plasma whose properties are described by pQCD. These two interpretations are both mutually exclusive and highly dependent upon the initial conditions of HIC.
Hydrodynamics. The stunning success of ideal relativistic hydrodynamics at RHIC as compared to its failure in lower energy machines [1132, 1133, 880, led to the proclamation of the creation of a perfect fluid at RHIC [1134, 1135, 1136, In HIC particle spectra are often conveniently reported as

$$
\begin{equation*}
\frac{d N^{h}}{d p_{T}}\left(p_{T}, \phi, N_{\text {part }}\right)=\frac{d N^{h}}{d p_{T}}\left(p_{T}, N_{\text {part }}\right)\left(1+2 v_{2}^{h}\left(p_{T}, N_{\text {part }}\right) \cos 2 \phi+\ldots\right), \tag{5.190}
\end{equation*}
$$

where $\phi$ is the angle of the observed particle with respect to the semiminor axis of the overlap region; see figure 5.92 (a). As pictured in figure 5.92 (a) the $v_{2}^{h}$ develops from pressure gradients that build up as a result of the spatial anisotropy created in the initial overlap of the two nuclei.

The nearly ideal fluid flow as surmised from hydrodynamics is exciting because the extracted value of $\eta / s$, the shear viscosity to entropy ratio, is smaller than for any other known substance [1137. From a theoretical standpoint, this nearly ideal flow is a huge success for string phenomenology: the lower bound for $\eta / s$ in a strongly-coupled liquid as computed using the AdS/CFT correspondence is $1 / 4 \pi$, in natural units. This value of $1 / 4 \pi \simeq 0.1$ should be compared to the naive estimate from $\mathrm{pQCD}, \eta / s \sim 1$. Conservative


Figure 5.93. (a) A plot of the early success of pQCD energy loss calculations in describing $R_{A A}\left(p_{T}\right)$, Eq. 5.191 (b) Cartoon of the energy loss from a high- $p_{T}$ parton in the QGP medium. The longer the pathlength $L$ the greater the energy loss: the spatial anisotropy manifests as a suppression anisotropy, which is represented by $v_{2}^{h}$. (c) pQCD ( $\Delta E \sim L^{2}$ ) energy loss significantly underpredicts the anisotropy while AdS/CFT $\left(\Delta E \sim L^{3}\right)$ loss is consistent. The simultaneous description of $R_{A A}$ and $v_{2}$ seems to require both $L^{3}$ energy loss and a CGC-like initial state. figures adapted from 1140, 884.
estimates of the extracted value of $\eta / s$ from comparison between theoretical calculations and experimental data yield $\eta / s \sim 0.1-0.5$ [1137]. Hydrodynamics is a set of partial differential equations: initial conditions, for which hydrodynamics can tell us nothing, must be supplied. Figure 5.92 (b), in which a $2+1 D$ viscous hydrodynamics calculation is compared with data, shows the at least factor of 2 uncertainty in the extracted value of $\eta / s$ that arises from the poorly constrained mean value of the initial geometry. The uncertainty from fluctuations [1138], in which hot and cold spots appear in the initial conditions, might also be very large [1139]. This very large range of $\eta / s$ means that one cannot definitively claim that the medium is better understood as strongly coupled and near the lower bound set by AdS/CFT or weakly coupled, with pQCD providing a good physical description.
High-pT Physics. Originally, high- $p_{T}$ particles were hoped to provide a tomographic probe of the QGP medium produced at RHIC. Jet tomography, then, would provide a means, independent of hydrodynamics, for determining many medium properties; most important, jet tomography could be a tool to investigate the initial geometry of the HIC. While early work showed great promise, see figure 5.93 (a), there are several observables for which the perturbative energy loss calculations do not provide a good description of the data (see, e.g., figure 5.93 (c)). There is currently not much theoretical control over the inmedium energy loss experienced by high- $p_{T}$ partons: different assumptions about the best physics approximations have yielded very different energy loss calculations (see, e.g., [1141, (1011), and all these calculations suffer from large, mostly unquantified uncertainties due to simplifying mathematical approximations [1142]. Nevertheless, qualitatively fascinating discoveries can be made from high- $p_{T}$ observables. In particular, one may compare the results of strong coupling calculations derived using the AdS/CFT correspondence to those derived using traditional pQCD methods; in this way, energy loss holds out the possibility of rigorously investigating, independent of hydrodynamics, whether RHIC creates a stronglycoupled perfect fluid or a weakly-coupled plasma.

High-energy particle spectra are often reported as normalized by the $p+p$ spectrum multiplied by $N_{\text {coll }}\left(N_{\text {part }}\right)$, where $N_{\text {coll }}\left(N_{\text {part }}\right)$ is the expected number of $p+p$-like hard
collisions in an $A+A$ collision with a given number of participants:

$$
\begin{equation*}
R_{A A}^{h}\left(p_{T}, \phi, N_{\text {part }}\right)=\frac{d N_{A A}^{h}}{d p_{T}}\left(p_{T}, \phi\right) / N_{\text {coll }}\left(N_{\text {part }}\right) \frac{d N_{p p}^{h}}{d p_{T}}\left(p_{T}\right), \tag{5.191}
\end{equation*}
$$

where $h$ is the measured hadron species and $\phi$ is the same angle as was defined in the discussion of hydrodynamics. This ratio is also often reported as a Fourier expansion, with $v_{2}^{h}$ again representing twice the first Fourier coefficient (the same $v_{2}^{h}$ as in hydrodynamics). However the physical understanding of the origin of the high- $p_{T} v_{2}^{h}$ is very different from the hydrodynamics physics which dominates the generation of the low- $p_{T} v_{2}^{h}$. For high$p_{T}$ observables, $v_{2}^{h}$ comes from high $-p_{T}$ partons traversing a medium asymmetric from the initial geometry: less energy loss occurs for partons traveling the short direction of the almond-shaped overlap region compared to those partons that travel the long direction. A cartoon of this physical picture is shown in figure 5.93 (b). The size of $v_{2}^{h}$ is then an entangled measure of the geometry of the medium and the pathlength dependence of the energy loss mechanism: perturbative elastic energy loss, which goes as $L^{1}$, produces less $v_{2}^{h}$ for a given geometry than perturbative inelastic energy loss, which goes as $L^{2}$, which produces less $v_{2}^{h}$ than strong-coupling energy loss, which, for light partons, goes as $L^{3}$ and as $\exp (-L)$ for heavy partons. $v_{2}^{h}$ is of particular interest because it was recently measured out to $p_{T} \sim 13 \mathrm{GeV}$, well beyond momentum scales where hadronization effects might be important. That the observed $v_{2}^{h}$ is significantly larger than that predicted by perturbative methods, shown in figure 5.93 (c), is perhaps the best high- $p_{T}$ experimental evidence that $\mathrm{AdS} / \mathrm{CFT}$, as opposed to pQCD, is the best approximation to the relevant physics at RHIC.

As the theoretical prediction of high- $p_{T} v_{2}^{h}$ comes directly from the azimuthal anisotropy of the QGP medium, knowledge and constraint of the initial geometry is crucially important for a rigorous scientific conclusion to be made: the sharper the produced medium the larger the $v_{2}^{h}$, regardless of energy loss mechanism. As one can see from figure 5.93, there are reasonable initial conditions for which no known energy loss calculation describes the data. And just as in hydrodynamics, fluctuations may play an important, even outsized, role.
Measuring the Initial State. From the above discussion it is clear that knowledge of the initial conditions at RHIC is crucial for interpreting the experimental data. The density of the charged and neutral matter density of nuclei at rest is well understood from diffraction pattern experiments (see, e.g., [1143]). Knowledge of the rest frame density of protons and neutrons in nuclei has been used extensively in estimating the initial matter density created in HIC. Matter production in HIC, though, depends on the distribution of quarks and, especially, gluons in the nuclear wavefunction. Below some value of Bjorken $x$ that is not yet precisely known, non-Abelian, non-linear QCD evolution effects become important. The (mostly) gluonic initial state medium at midrapidity at RHIC consists of particles of $x \sim p_{T} / \sqrt{ } s \sim 10^{-3}$, which is at the order of magnitude for which small- $x$ physics likely becomes relevant. Unfortunately the theory of small-x physics in $A+A$ collisions is very complicated, and current knowledge is incomplete. Additionally, the aforementioned theoretical calculations of $v_{2}^{h}$ are in fact most sensitive to the the quantitative shape of the edge of the initial nuclear overlap in HIC; it is just in this region that many of the theoretical tools developed for small-x physics study break down. It turns out, though, that through careful measurements, diffraction patterns may be measured at an electronion collider using deeply-virtual Compton scattering and vector meson production. These diffraction patterns, in turn, may be inverted to constrain the initial gluon and quark densities of the highly boosted nuclei. Fortuitously, these experimental measurements give
the most sensitive determination of these densities at the edge of the nucleus, the region of the overlap which hydrodynamics and energy loss calculations are most sensitive to.

### 5.15.2 Constraining initial conditions in $\mathrm{A}+\mathrm{A}$ collisions

Adrian Dumitru

Understanding small- $x$ gluon production in the initial state of relativistic $\mathrm{A}+\mathrm{A}$ collisions constrains the amount of additional entropy produced via "final-state" interactions such as parton thermalization / QGP formation [1144 and its subsequent hydrodynamic expansion. If these processes provide a significant contribution, then that should presumably show in the centrality dependence of the multiplicity in the final state: final state interactions should be much more prevalent for a head-on collision of two large nuclei than for a grazing shot or $\mathrm{p}+\mathrm{A}$ or (minimum bias) $\mathrm{p}+\mathrm{p}$ collisions. It is therefore very important to test models for initial particle production over a broad range of centralities - perhaps down to the level of $\mathrm{p}+\mathrm{p}$ collisions - in order to constrain entropy production due to thermalization and viscous hydrodynamic expansion (1145.

To compute the number of small- $x$ gluons released from the wavefunctions of the colliding nuclei, one frequently employs the $k_{\perp}$-factorization formalism [742, 1146],

$$
\begin{align*}
& \frac{d N}{d^{2} \mathbf{r}_{\perp} d y}=\mathcal{N} \frac{N_{c}}{N_{c}^{2}-1} \int \frac{d^{2} p_{\perp}}{p_{\perp}^{2}} \int^{p_{\perp}} d^{2} k_{\perp} \alpha_{s}\left(Q^{2}\right) \\
& \quad \times \phi_{A}\left(x_{1}, \frac{\left(\mathbf{p}_{\perp}+\mathbf{k}_{\perp}\right)^{2}}{4} ; \mathbf{r}_{\perp}\right) \phi_{B}\left(x_{2}, \frac{\left(\mathbf{p}_{\perp}-\mathbf{k}_{\perp}\right)^{2}}{4} ; \mathbf{r}_{\perp}\right), \tag{5.192}
\end{align*}
$$

where $N_{c}=3$ is the number of colors, and $p_{\perp}, y$ are the transverse momentum and the rapidity of the produced gluons, respectively. $x_{1,2}=p_{\perp} \exp ( \pm y) / \sqrt{s_{N N}}$ denote the lightcone momentum fractions of the colliding gluon ladders, $\sqrt{s_{N N}}$ is the collision energy, and typically one chooses $Q^{2}=\max \left(\left(\mathbf{p}_{\perp}+\mathbf{k}_{\perp}\right)^{2},\left(\mathbf{p}_{\perp}-\mathbf{k}_{\perp}\right)^{2}\right) / 4$. The normalization factor $\mathcal{N}$ can be fixed from peripheral collisions, where final-state interactions should be suppressed. It effectively also absorbs NLO corrections and the contribution from sea (anti-)quarks. The unintegrated gluon distribution $\phi$ is related to the dipole scattering amplitude in the adjoint representation, $N_{G}$, through a Fourier transform [1147]:

$$
\begin{equation*}
\phi\left(x, k_{\perp}^{2} ; \mathbf{r}_{\perp}\right)=\frac{C_{F}}{\alpha_{s}\left(k_{\perp}\right)(2 \pi)^{3}} \int d^{2} \mathbf{s}_{\perp} e^{-i \mathbf{k}_{\perp} \cdot \mathbf{s}_{\perp}} \nabla_{\mathbf{s}_{\perp}}^{2} N_{G}\left(x, s_{\perp} ; \mathbf{r}_{\perp}\right) . \tag{5.193}
\end{equation*}
$$

The multiplicity in heavy-ion collisions. Figure 5.94 (left) shows the centrality dependence of particle production for heavy-ion collisions at 200 GeV and 2760 GeV , respectively, obtained by integrating eq. (5.192) over the transverse overlap of the colliding nuclei. The unintegrated gluon distributions are solutions of the local (impact parameter independent) Balitsky-Kovchegov (BK) equation with running-coupling corrections according to the Balitsky prescription [751]. The impact parameter dependence is due entirely to the initial condition where it has been assumed that essentially $Q_{s}^{2}\left(x_{0} ; \mathbf{r}_{\perp}\right)=Q_{0}^{2} \sigma_{0} T_{A}\left(\mathbf{r}_{\perp}\right)$ increases in proportion to the thickness of the nucleus ( $Q_{0}$ and $\sigma_{0}$ denote constant scales; for details see ref. [896). Neglecting the impact parameter dependence of the dipole scattering amplitude $N_{G}$ in a nucleon relies on the scale separation $R_{A} \gg R_{N} \gg Q_{s}^{-1}$ where $R_{A}$ is the size of the overlap region in the collision 1150 .


Figure 5.94. Left: Centrality dependence of the multiplicity at 200 GeV and 2760 GeV , respectively, from $k_{\perp}$ factorization with running-coupling BK unintegrated gluon distributions (see [896] for details). PHOBOS data: 891] $(\mathrm{Au}+\mathrm{Au})$, 1148 , $(\mathrm{Cu}+\mathrm{Cu})$; ALICE data from ref. 894]. Right: $v_{2} / \varepsilon$ versus the transverse particle density [1149] $v_{2} / \varepsilon_{\mathrm{CGC}}$ has been scaled by $1 / 2$ for better visibility.

Apparently, the model calculation describes both the centrality and the energy dependence of particle production fairly well. If so, this constrains final-state entropy production and correlates the thermalization time and the shear viscosity to entropy density ratio: extremely rapid thermalization and/or $\eta / s \gtrsim 0.3$ would be excluded by stringent entropy production bounds [1145].

Several caveats remain. As already mentioned above, the absolute normalization of the gluon density at small $x$ (alternatively, the factor $\mathcal{N}$ in the $k_{\perp}$ factorization formula) can be fixed in practice only from very peripheral $\mathrm{A}+\mathrm{A}$ or $\mathrm{p}+\mathrm{p}$ collision: 9 . For $\mathrm{p}+\mathrm{p}$ collisions, however, the impact parameter dependence of the dipole scattering amplitude over distance scales $\sim R_{N}$ can not be neglected, see for example ref. [1151.

Furthermore, it may be important to consider in more detail the structure of running coupling corrections to the $k_{\perp}$-factorization formula (5.192) [897] and the effect of a full NLO treatment of BK evolution. Indeed, if such corrections modify the centrality dependence of particle production in $\mathrm{A}+\mathrm{A}$ collisions then they will also affect entropy production constraints and thus the fundamental understanding of the thermalization processes and time scales as well as estimates of the shear viscosity of thermal QCD.
The eccentricity in heavy-ion collisions. Other quantities of relevance for the interpretation of heavy-ion collisions exhibit even greater sensitivity to the actual distribution of produced gluons in the transverse $\mathbf{r}_{\perp}$ plane than its integral $d N / d y$. A collision of two heavy ions at non-zero impact parameter, neglecting fluctuations of the local density of participant nucleons, leads to a momentum asymmetry called "elliptic flow", $v_{2} \sim\langle\cos 2 \phi\rangle$, as described in section 5.15.1. In the absence of any scales (such as the freeze-out temperature $T_{f}$, the phase transition temperature $T_{c}$, or a non-vanishing mean free path $\lambda$ ), hydrodynamics predicts that $v_{2}$ is proportional to the eccentricity $\varepsilon$ of the overlap area [1152], $\varepsilon=\left\langle y^{2}-x^{2}\right\rangle /\left\langle y^{2}+x^{2}\right\rangle$. The average is taken with respect to the distribution of produced gluons in the transverse $x-y$ plane. Clearly, $\varepsilon$ involves large cancellations of the contributions of gluons produced near the center $r_{\perp} \sim 0$ of the overlap zone and so is more sensitive to particle production in the periphery.

A simple geometry based initial condition assumes that by analogy to the Glauber model for soft particle production $d N / d y d^{2} r_{\perp} \sim \rho_{\text {part }}^{\text {ave }}\left(r_{\perp}\right) \equiv\left(\rho_{\text {part }}^{A}\left(r_{\perp}\right)+\rho_{\text {part }}^{B}\left(r_{\perp}\right)\right) / 2$, where $\rho_{\text {part }}^{i}$

[^282]is the density of participants of nucleus $i$ per unit transverse area. High-density QCD (the "Color-Glass Condensate") predicts a somewhat different distribution of gluons in the transverse plane, corresponding to a higher eccentricity $\varepsilon$. In particular, in the " $\mathrm{p}+\mathrm{A}$ limit" when one of the nuclei is very dense while the other is dilute, the number of produced particles is proportional only to the density of the dilute collision partner, whose partons add up linearly. Hence, in the reaction plane, $d N / d y d^{2} r_{\perp} \sim \min \left(Q_{s, A}^{2}, Q_{s, B}^{2}\right) \sim \min \left(\rho_{\text {part }}^{A}, \rho_{\text {part }}^{B}\right)$ drops more rapidly as one moves towards the edge of the overlap zone than $d N / d y d^{2} r_{\perp} \sim$ $\rho_{\text {part }}^{\text {ave }} 1153$. Thus, a higher eccentricity is a generic effect due to a dense target or projectile. Specific numerical estimates rely on an accurate determination of the unintegrated gluon distribution, however. Ref. [896] finds that the energy dependence of $\varepsilon$ from RHIC to LHC is very weak.

Figure 5.94 (right) shows the elliptic flow $v_{2}$ measured in heavy-ion collisions at RHIC scaled by the eccentricity $\varepsilon$ of the overlap zone 1149 . As already mentioned above, in the absence of any scales such as a non-zero mean free path, $v_{2} / \varepsilon$ would be independent of the transverse density of particles. Indeed, if the $v_{2}$ data is scaled by the eccentricity obtained from a CGC model implementation then the required breaking of scale invariance is lower than for purely geometry based (Glauber-like) initial conditions. Actual solutions of viscous hydrodynamics (for $v_{2}$ ) appear to confirm this simple observation in that the slope of $v_{2} / \varepsilon$ versus transverse density is sensitive to the distribution of produced particles [1154.

More recent studies attempt to understand also the relation of higher moments of anisotropic flow $v_{n}$ to corresponding moments of the initial eccentricity $\varepsilon_{n}-$ such as the "triangularity" [1155, 1156, 1157, 883, 1158, which is non-zero because of fluctuations of the large- $x$ sources in the transverse impact parameter plane before the collision. A quantitative interpretation of the "response" $v_{n}$ of the Quark-Gluon Plasma medium to the initial geometry will also rely on a good understanding of particle production in high-energy QCD.

### 5.15.3 Particle production at low- $x$ and gluon saturation: from $p+A$ to $e+A$

## Kirill Tuchin

In the beginning of the RHIC era, the $p(d)+A$ program was perceived as merely a useful baseline reference for the heavy-ion program. It very soon turned out that due to a wise choice of colliding energy, RHIC probes the transition region to a new QCD regime of gluon saturation. While the first hints of gluon saturation were observed in DIS experiments at HERA, it is fair to say that gluon saturation was discovered in $d A$ collisions at RHIC. At present, as we are heading toward the era of EIC, it is important to review what we have learned at RHIC and how it can be used to optimize the EIC program. The purpose of this section is to review phenomenological studies of gluon saturation at RHIC.

The reason why $p A$ and $e A$ high energy physics programs are closely related is provided by the Pomerantchuk theorem, which states that all high energy scattering processes are mediated by the exchange of a collective gluon state - known as a Pomeron - that has vacuum quantum numbers. For this reason, inclusive processes in both programs share many similarities in the low $x$ region. The main distinction arises from the difference in the characteristic scales of the projectile: in protons it is a soft scale $\Lambda$, while in virtual photons, it is the photon virtuality $Q^{2}$, which depends on the electron kinematics. A possibility to control the $Q^{2}$ is a great advantage of DIS. In particular, it allows one to study the total cross sections/structure functions. However, in practice, the requirement to keep $x$ low
significantly restricts the range of $Q^{2}$, s available for low $x$ studies.
The relation between $p A$ and $e A$ scattering at low- $x$ becomes particularly apparent in the framework of the dipole model [737]. In the dipole model, the cross section for $e A \rightarrow X$ or $p A \rightarrow X$ scattering, where $X$ is an arbitrary final state, can be represented as

$$
\begin{equation*}
d \sigma_{p\left(\gamma^{*}\right)+A \rightarrow X}=\int d^{2} r_{\perp} \Phi^{p\left(\gamma^{*}\right)}\left(r_{\perp}\right) d \sigma_{\mathfrak{D}+A \rightarrow X}\left(r_{\perp}\right) \tag{5.194}
\end{equation*}
$$

where $\mathfrak{d}$ stands for color dipole (letter $d$ is reserved for deuteron) of size $r_{\perp}$ in the transverse plane. Eq. (5.194) is based on the separation of scales: the interaction length $\ell_{i} \sim R_{A}$ (in the target rest frame) is much smaller than the coherence length $\ell_{c}=\gamma / M_{N}$, where $\gamma \gg 1$ is the Lorentz factor and $M_{N}$ is the nucleon mass. $\Phi^{p\left(\gamma^{*}\right)}\left(r_{\perp}\right)$ is the light-cone "wave function" describing the Fourier decomposition of a projectile into dipoles; it can be calculated in QED (for $\gamma^{*}$ ), or modeled (for proton), see e.g. [1159, 1160. The main theoretical concern in low $x p A / e A$ scattering is calculation of the dipole-nucleus cross section, which is universal for both processes. With this observation in mind, we are going to consider some of the $p A$ processes at RHIC that are of relevance for low- $x$ physics at EIC.
Inclusive hadron production: $p+A \rightarrow h+X$. The cornerstone for phenomenological applications of the Color Glass Condensate (CGC), which is the theory of gluon saturation, is the factorization theorem proved in [1147, where the cross section was derived that resums all leading logarithmic contributions $\alpha_{s} \ln (1 / x) \sim 1$ (LLA) for a heavy nucleus in the quasi-classical limit $\alpha_{s}^{2} A^{1 / 3} \sim 1$. A similar result was reported in [1161, 1162, 1163]. One does not expect that any of the hard perturbative QCD (hpQCD) factorizations apply in this case because higher twist interactions of valence quarks and gluons give contributions of order unity. Nevertheless, despite the fact that individual diagrams break factorization in covariant and light-cone gauges, the final re-summed expression can be cast in the $k_{T}$-factorized form. Unlike in hpQCD, the physical quantity that is factorized - the unintegrated gluon distribution $\varphi\left(x, Q^{2}\right)$ - can be calculated perturbatively owing to the existence of a hard scale $Q_{s} \gg \Lambda_{\mathrm{QCD}}$. Another surprising fact is that contrary to naive expectations, $\varphi\left(x, Q^{2}\right)$ is related not to the momentum space Fourier-image of the nucleus gluon-field correlation function $\left\langle A_{\perp}\left(0_{\perp}\right) \cdot A_{\perp}\left(x_{\perp}\right)\right\rangle$, but rather to the Fourier-image of $\nabla_{r}^{2} N\left(r_{\perp}, b_{\perp}, y\right)$, where $N\left(r_{\perp}, b_{\perp}, y\right)$ is the imaginary part of the forward elastic scattering amplitude of a color dipole of size $r_{\perp}$ at impact parameter $b_{\perp}$ and rapidity $y=\ln (1 / x)$ in the heavy nucleus. Although the inclusive gluon production in $p A$ collisions is the only known case were $k_{T}$-factorization holds, factorization of the multipoles in the transverse coordinate space is a general feature of the low- $x$ cross sections. It must be stressed that this multipole factorization does not imply hpQCD factorizations ( $k_{T}$ or collinear ones) and neither opposite is generally true.

The $k_{T}$-factorization formula derived in [1147] led to successful phenomenology of inclusive hadron production in $d A$ collisions at RHIC, where the suppression of hadrons at forward rapidities and Cronin enhancement at mid-rapidity were qualitatively predicted [1164, 1165] and then quantitatively described in the CGC framework [1166, 1167, 1168]. The production of valence quarks in the forward direction gives an important contribution to inclusive hadron production at large- $x$ of the proton and was discussed in [1169, 1170, 1171].

By integrating the gluon spectrum over $p_{\perp}$, one arrives at the total hadron yield as a function of rapidity $y$. It is rather weakly dependent on the details of the gluon distributions. Therefore, a simple model suggested in [1172] is able to describe inclusive hadron yield with remarkable accuracy.

Open charm (beauty) production: $\boldsymbol{p}+\boldsymbol{A} \rightarrow \boldsymbol{D}+\boldsymbol{X}$. The production of heavy quarks in $p A$ collisions at low- $x$ was calculated in [1173, 905, 1174]. One expects that the hpQCD factorization is applicable if the saturation momentum is much smaller than the quark mass $m$ [1175]. At RHIC, $Q_{s} \sim m$ for charm and bottom, hence factorization is broken in both cases. Indeed, analysis of [1176] indicates that semi-classical calculations of 905 disagree with $k_{T}$-factorization by about $10 \%$ at the $t$-channel gluon transverse momenta around $m$. hpQCD factorization is restored in the kinematic region where the operator product expansion is applicable, i.e. at transverse momenta much higher than the saturation momentum.

The phenomenology of open heavy quark production at RHIC was developed in [1177], where it was found that the production pattern of heavy quarks is qualitatively similar to that of light quarks and gluons, although the magnitude of nuclear effects (Cronin and suppression) slowly decrease with increasing quark mass. These qualitative features are in good agreement with preliminary data.
Inclusive production of $J / \Psi: p+A \rightarrow J / \Psi+X$. In addition to the scales $\ell_{i}$ and $\ell_{c}$ mentioned earlier, the production of a charmonium state is characterized by another scale: formation length $\ell_{f}=\gamma / \Delta M$, where $\Delta M$ is its binding energy. The key theory observation is strong ordering of the scales at high energies: $\ell_{i} \ll \ell_{c} \ll \ell_{f}$ [977, 1178]. Consequently, we can distinguish three stages of $J / \Psi$ production. (i) $g^{*} \rightarrow c \bar{c}$ described by the light-cone amplitude $\psi^{g}\left(k_{\perp}, z\right)$ often referred to as gluon's light-cone wave function, (ii) interaction of the gluon or the $c \bar{c}$ with the target depending on whether the splitting has occurred after or before the interaction, and (iii) formation of charmonium wave function. Unlike stages (i) and (ii), which can be described using perturbation theory owing to the weakness of the strong interaction at the $J / \Psi$-mass scale, stage (iii) is non-perturbative because $\Delta M \ll M$. This, however, does not preclude us from using perturbation theory for calculating the $J / \Psi$ production cross section, since the fragmentation process is independent of energy and atomic weight $\left(\ell_{f} \gg R_{A}\right)$. In other words, fragmentation happens in the vacuum long after any interaction with the target.

Thus, the problem of calculating the $J / \Psi$ production cross-section reduces to the calculation of the cross section of $\mathfrak{d}+A \rightarrow\left[c \bar{c}\left(1^{--}\right)\right]+X$ dipole-nucleus scattering. This calculation was done in [1179, 1180. Note, that interaction depends on the quantum state of the $c \bar{c}$ pair, which must be in the $1^{--}$color singlet state. Therefore, only those higher twist contributions may be taken into account that lead to this quantum state, and which are also enhanced by $\alpha_{s}^{2} A^{1 / 3} \sim 1$. At the lowest order in $\alpha_{s}$, the projectile gluon in the proton wave-function has two interaction possibilities: (i) leading twist processes $g+g \rightarrow J / \Psi+g$, which is of order $\mathcal{O}\left(\alpha_{s}^{5} A^{1 / 3}\right)$ and (ii) higher twist process $g+g+g \rightarrow J / \psi$ (initial gluons come from different nucleons), which is of the order $\mathcal{O}\left(\alpha_{s}^{6} A^{2 / 3}\right)$. Since $\alpha_{s}^{2} A^{1 / 3} \sim 1$, the higher twist mechanism (ii) is parametrically enhanced. Notice, that this leading contribution explicitly breaks $k_{T}$-factorization as it is proportional to $x G\left(x_{1}\right)\left[x G\left(x_{2}\right)\right]^{2}$. Results reported in [1179, 1180] show strong coherence effects consistent with expectations of CGC theory.
Electromagnetic probes. The main advantage of electromagnetic probes, such as photons and dileptons, is that they are directly observable without an intermediate hadronization process, in contrast to quarks and gluons. Therefore, they are a cleaner probe of low$x$ nuclear matter. Their disadvantage is a low production rate due to the smallness of electromagnetic coupling. Prompt photon production in $p A$ collisions was considered in [1181] through the process $q A \rightarrow \gamma q X$. The production of di-leptons in a similar process $q A \rightarrow l^{+} l^{-} q X$ was addressed in [1182, 1183, 1184]. At higher energies, gluons become
much more abundant than quarks in the central rapidity region which implies that photon (dilepton) production will go via the process $g^{*} A \rightarrow q \bar{q} X \gamma\left(l^{+} l^{-}\right)$. It is suppressed by $\alpha_{s}$ but enhanced by a positive power of energy. There have been no detailed phenomenological studies of electromagnetic probes in $p A$ collisions at RHIC.
Double inclusive hadron production and correlations. Azimuthal correlations are an important tool to investigate properties of QCD at low $x$. In 1185 it was proposed that azimuthal correlations of hadrons produced at large rapidity separation $(\Delta y \gg 1)$ may be depleted due to a quasi-classical nature of the saturated gluon fields. Unfortunately, accurate theoretical calculations in the region of large but finite $\Delta y$ are challenging as they must involve complicated NLO BFKL effects. Important progress has been made in the investigation of azimuthal correlations at smaller $\Delta y$.

It has been suggested that correlations at small $\Delta y$ in the forward direction can be effectively used to study gluon saturation [1186], where the forward direction corresponds to low- $x$ of the nucleus where saturation effects are strongest. Theory predicts that back-toback correlations are suppressed due to gluon saturation. Phenomenological models based on the CGC were suggested in [1186, (1187] and [1188] and rely on different approximations. An approach of [1186, 1187] is based on the dipole model [737] in which double inclusive gluon [1189], quark-anti-quark [1173, 905, [1174] and valence quark-gluon [1186] cross sections were calculated. Another approach [1188] is based on an approximate $k_{T}$-factorization and relies on calculating double-inclusive production based on NLO BFKL [1190, 1191 .

Both models give a reasonable quantitative description of experimental data. However, in order to use azimuthal correlations to study low- $x$ physics in the most effective way, work remains to be done to reconcile the existing approaches and reduce model-dependencies in calculations. Measurements of forward azimuthal correlations in $e A$ will have a clear advantage over that in $p A$ due to much better theoretical control of the projectile current. Diffraction. One of the most sensitive probes of low- $x$ QCD is diffraction. This is because scattering in the high energy limit of QCD is mediated by the same collective gluon state (Pomeron) as the diffractive scattering. Saturation effects on diffractive processes in $p A$ collisions were investigated in [1159, 1192, 1193, 1160, 1194 where the main focus was on diffractive hadron production. (In [1195, 1196 this work was extended to DIS).

In diffraction on nuclear targets, it is important to distinguish two processes: coherent and incoherent diffraction, depending on the final state of the target. Coherent diffractive hadron production in $p A$ collisions is a process $p+A \rightarrow X+h+[L R G]+A$, where $[L R G]$ stands for Large Rapidity Gap. Coherent diffractive production exhibits a much stronger dependence on energy and atomic number than the corresponding inclusive process. Indeed, the diffractive amplitude is proportional to the square of the inelastic one. At asymptotically high energies, coherent diffractive events are expected to constitute up to a half of the total cross section, the other half being all inelastic processes. Therefore, coherent diffraction is a powerful tool for studying the low- $x$ dynamics of QCD.

In all phenomenological applications of the CGC formalism, one usually relies on the mean-field approximations in which only the lowest order Green's functions are relevant. Although corrections to the mean-field approximation, i.e. quantum fluctuations about the classical solution, are assumed to be small in $p A$ collisions at RHIC, their detailed phenomenological study is absent. An observable that is directly sensitive to quantum fluctuations is incoherent diffraction: $p+A \rightarrow X+h+[L R G]+A^{*}$, where $A^{*}$ denotes excited nucleus that subsequently decays into a system of colorless protons, neutrons and nuclei debris. Incoherent diffraction measures fluctuations of the nuclear color field. Calculations show that unlike the nuclear modification factor for coherent diffractive gluon production,
the nuclear modification factor for incoherent diffraction is not expected to exhibit a significant rapidity and energy dependence [1194]. Therefore, the two diffractive processes can in principle be experimentally distinguished and yield unique information about low- $x$ QCD. Unfortunately, the study of diffraction in $p A$ collisions at RHIC is a virgin subject in part due to technical difficulties associated with measurements at very small forward angles.
Instead of a summary. Studying particle production in DIS at low $x$ has two main advantages: (i) one has much better theoretical understanding of the forward kinematic region owing to the weakness of the QED coupling and (ii) new kinematic regions open up for investigation depending on values of momentum scales $Q^{2}, k_{\perp}^{2}$ and $Q_{s}^{2}$, where $Q^{2}$ is photon virtuality, $Q_{s}^{2}$ is saturation scale and $k_{\perp}$ is transverse momentum of produced hadron.

### 5.15.4 Small-x dynamics in ultraperipheral heavy ion collisions at the LHC

Mark Strikman

Experiments at HERA have demonstrated that reactions with quasi real photons provide an effective tool of probing pQCD which complements studies of DIS processes. In the near future it will be possible to extend these studies to ultra-high energy photon - nucleus collisions via the study of ultra-periperal collisions (UPCs) of heavy ions (protons and ions) at the LHC. The feasibility and the possible reach of these investigations was explored in a five year long study undertaken by the collaboration of theorists and experimentalists. The results of the study were published as a volume of Physics Reports [979]. Due to the high energy of the colliding nuclei and very good acceptance of the CMS and ATLAS detectors at large rapidities, UPCs at the LHC allows to study a wide range of the processes sensitive to the small-x dynamics for $W_{\gamma N} \leq 1-2 \mathrm{TeV}$. This would extend the $x$ range probed at HERA down by at least by a factor of ten. A further advantage


Figure 5.95. The kinematic range in which UPCs at the LHC can probe gluons in protons and nuclei in quarkonium, di-jet and di-hadron production. For comparison, the kinematic ranges for $J / \psi$ at RHIC, $F_{2}^{A}$ and $\sigma_{L}^{A}$ at eRHIC and $Z^{0}$ hadroproduction at the LHC are also shown. for the search for non-linear effects will be the use of the nuclear targets.

The kinematic range for which studies of several processes of interest will be feasible is presented in figure 5.95 (taken from [979]) as a function of $x$ and $Q$ which is the typical gluon virtuality which, as the transverse momentum of the jet or leading pion, sets the scale for dijet and $\pi \pi$ production respectively. The typical gluon virtuality scale for exclusive quarkonium photoproduction is shown for $J / \psi$ and $\Upsilon$. Below we list some of the directions of the planned studies.

Dijet production. Dijet production in the discussed kinematic range is dominated by photon - gluon fusion. Estimates of the counting rates including cuts due to the acceptance of the CMS detector were performed in [1197]. It was found that measurements of the nuclear gluon pdfs will be feasible down to $x \sim 10^{-4}$ via study of several channels: dijet, charm, beauty jets, providing a number of cross checks. Use of the zero degree calorimeters (ZDCs) will also allow the separation of diffractive events and hence measure the nuclear gluon diffractive pdfs in the same kinematics. Hence, it will be possible to test a prediction of the leading twist theory of nuclear shadowing that the probability of the gluon induced coherent diffraction at large $p_{T}$ and small $x$ should be of the order $10-15 \%$ [812].

The cutoff $p_{t}($ jet $) \geq 6-8 \mathrm{GeV} / \mathrm{c}$ (necessary for selecting dijet production) reduces non-linear effects in dijet production. The parameter which governs non-linear effects is $R_{N L}=C_{F}^{2} \alpha_{s}(Q) x G_{T}\left(x, Q^{2}\right) / \pi r_{T}^{2} Q^{2}$, where $C_{F}^{2}$ is the Casimir operator, equal to $4 / 3$ for $q \bar{q}$ and 3 for $g g$, and $r_{T}$ is the transverse area of the target. For the smallest $x, p_{T}$ corner, $R_{N L}$ for the UPC processes $R_{N L}$ is about the same as for $F_{2 A}\left(x, Q^{2} \sim 2-4 \mathrm{GeV}^{2}\right)$ for the lowest $x$ which could be reached at the EIC.

It will be also possible to reach larger $R_{N L}$ at smaller virtualities and $x \sim 10^{-4}$ using leading pion production in the central detectors $|y| \leq 2.4$ - see dashed area in figure 5.95, This is a kinematics similar to the production of two forward pions in $\mathrm{d}+\mathrm{Au}$ collisions at RHIC. Within the mechanism of fractional energy losses [981, 1198, one expects a strong suppression of the two pion yield as compared to the single pion yield which would allow one to perform clean tests of the onset of the black disk regime ( BDR ).

Another sensitive probe of the onset of BDR would be exclusive diffractive production of two jets in the process $\gamma+\mathrm{A} \rightarrow 2$ jets +A . In the case of light quark jets, this process is strongly suppressed in the pQCD regime, while it is a dominant contribution to the diffraction mechanism in the BDR 981 .

The interaction of small dipoles with nuclear media. In the leading twist approximation, the suppression of onium coherent production is given by the square of the ratio of the gluon densities in the nucleus and the proton gluon pdfs. It will be feasible to investigate the suppression of coherent $J / \psi, \Upsilon$ production in nucleus-nucleus collisions down to $x \sim m_{\text {onium }} / 2\left(E_{A} / A\right)$ corresponding to production at the central rapidities. At rapidities away from zero, photons of smaller energies dominate in the production of $J / \psi$, making it very difficult to probe smaller x for virtualities $\sim 3 \mathrm{GeV}^{2}$ characteristic for $J / \psi$ coherent photoproduction. However, the use of incoherent diffractive onium production appears to solve this problem as one can use production of soft neutrons to determine which of the nuclei emitted a photon and which was involved in the strong interaction [979]. As a result, there is a potential for probing $J / \psi$ production down to $x \sim 10^{-6}$, see figure 5.95.

A complementary method of tracking a small dipole through the nuclear media will be provided by the $J / \psi$ production in the $-t \geq$ few $\mathrm{GeV}^{2}$ process $\gamma+A \rightarrow J / \psi+$ rapidity gap +Y [982]. It is possible in this case to select the kinematics where $x_{g}$ of the gluon involved in the hard process is $x_{g} \geq 0.01$. In this case, scattering at central impact parameters dominates and one can probe the propagation of a small dipole through $\sim 10 \mathrm{fm}$ of the nuclear media up to $W_{\gamma N} \sim 1 \mathrm{TeV}$.

In conclusion, it appears that UPC studies to be performed at the LHC in the next few years will allow for the search of several signals of the onset of the BDR. However, it will not be possible to perform a precision scan of the range of moderate $Q^{2}$ sensitive to the transition between non-linear and linear regimes in the $x$ range to be covered by the EIC. Hence the UPC - LHC and EIC programs will nicely complement each other.

## Chapter 6

## Electroweak physics

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### 6.1 Electroweak physics at the EIC

Krishna Kumar, Yingchuan Li, William J. Marciano

### 6.1.1 Introduction

The $S U(3)_{C} \times S U(2)_{L} \times U(1)_{Y}$ standard model of particle physics has been extremely successful in describing strong and electroweak interactions. Its unbroken gauge symmetry, $S U(3)_{C}$ or Quantum Chromodynamics (QCD), taken on its own, represents a "perfect theory"' with no arbitrary free parameter. Nevertheless, it beautifully encompasses all the basics of strong interactions: quark confinement, chiral symmetry breaking, asymptotic freedom, etc. The electroweak sector is potentially much more mutable. In addition to its, as yet, undiscovered Higgs scalar remnant of $S U(2)_{L} \times U(1)_{Y}$ symmetry breaking, it contains many arbitrary free masses, couplings and mixing angles. They are accommodated but not understood at a deep level. Questions such as: why parity violation, why 3 generations of quarks and leptons? etc suggest that simplifying principles must await future new discoveries. However, precision measurements and searches for rare phenomena still have important roles to play. They have the capability of indirectly probing scales of physics beyond collider facilities and expanding the horizons of electroweak physics.

The EIC is being proposed mainly for the study of strong interactions but also has a unique ability to measure parity violating structure functions involving $W^{ \pm}$and $Z$ boson mediated interactions. The high energy and luminosity combined with polarized electrons and protons as well as a variety of heavy ion targets will provide a wealth of data in an area never explored before.

Two EIC capabilities for electroweak measurements, outlined in table 6.1, are: 1) Precision measurements of the weak mixing angle over a broad range in $Q^{2}$ and 2) Searches for $e \rightarrow \tau$ flavor changing conversion. For the former, we show how parity violating, right-left, deep-inelastic polarized $e p$ and $e d$ asymmetries can be used to precisely determine the running $\sin ^{2} \theta_{W}(Q)$ as a function of $Q^{2}$. The comparison of those measurements with precision values obtained from other lower energy or Z-pole studies can be used to find hints of "new physics". Alternatively, the overall World average of $\sin ^{2} \theta_{W}$ can be compared with precisely determined quantities such as $\alpha_{E M}, G_{F}, m_{Z}$, and $m_{W}$ to test the SM at the quantum loop level and probe "new physics" effects. In the case of $e-\tau$ conversion, the $e p \rightarrow \tau X$ reaction is examined, including isolation cuts and $\tau$ identification. First estimates suggest that backgrounds are under control and the high luminosity goals of the EIC allow the search of reactions well beyond HERA sensitivities.

| Deliverables | Observables | What we learn | Phase I | Phase II |
| :---: | :---: | :---: | :---: | :---: |
| Weak mixing | Parity violating | physics behind EW | good precision | high precision |
| angle | asymmetries in <br> $e p$ - and $e d$-DIS | symmetry breaking <br> \& BSM physics | over limited <br> range of scales | over wide range <br> of scales |
| e- $\tau$ conversion | ep $\rightarrow \tau, \mathrm{X}$ | flavour violation <br> induced by BSM <br> physics | challenging | very promising |

Table 6.1. Science Matrix for Electroweak physics at an EIC.

# 6.2 The weak mixing angle via polarized electron scattering asymmetries 

Krishna Kumar, Yingchuan Li, William J. Marciano, Seamus Riordan

### 6.2.1 Introduction

The nature of spontaneous gauge symmetry breaking implies that the masses and couplings of weak gauge bosons $W$ and $Z$ are related by natural lowest order relations $\sin ^{2} \theta_{W}^{0}=e_{0}^{2} / g_{0}^{2}=1-m_{W}^{0}{ }^{2} / m_{Z}^{0}$. The weak mixing angle plays a central role in those correlations. In the context of the Standard Model (SM) as a complete stand alone theory, the renormalized weak mixing angle is related to the other precisely measured quantities

$$
\begin{align*}
\alpha^{-1} & =137.03599959(40)  \tag{6.1}\\
G_{\mu} & =1.1663788(7) \times 10^{-5} \mathrm{GeV}^{-2} \\
m_{Z} & =91.1871(21) \mathrm{GeV}
\end{align*}
$$

via

$$
\begin{equation*}
\sin ^{2} 2 \theta_{W}\left(m_{Z}\right)_{\overline{M S}}=\frac{4 \pi \alpha}{\sqrt{2} G_{\mu} m_{Z}^{2}\left[1-\Delta \hat{r}\left(m_{t}, m_{H}\right)\right]} \tag{6.2}
\end{equation*}
$$

where $\Delta \hat{r}$ denotes loop corrections that depend on the top quark and Higgs masses while the renormalized weak mixing angle is defined by modified minimal subtraction $\overline{M S}$ [1199, 1200. The value of $\sin ^{2} 2 \theta_{W}\left(m_{Z}\right) \overline{M S}$ can be determined from parity violating asymmetries and other weak interaction measurements. A comparison of the parameters in equation 6.2 at a high level of precision was used in the past to constrain the top quark mass (before its discovery) and more recently, to provide an upper bound on the Higgs boson mass, the missing particle of the SM. After the Higgs mass is directly measured, equation 6.2 will be used to probe for "new physics" effects at the tree or loop level.

Incorporating $m_{W}=80.398(25) \mathrm{GeV}$ via

$$
\begin{equation*}
\sin ^{2} \theta_{W}\left(m_{Z}\right)_{\overline{M S}}=\frac{\pi \alpha}{\sqrt{2} G_{\mu} m_{W}^{2}\left[1-\Delta r\left(m_{Z}\right)_{\overline{M S}}-0.0085 S-\mathcal{O}(1) m_{W}^{2} / m_{W^{*}}^{2}\right]}, \tag{6.3}
\end{equation*}
$$

with $\Delta r\left(m_{Z}\right)_{\overline{M S}}=0.0696(2)$ representing loop corrections insensitive to $m_{t}$ and $m_{H}$, one has another handle on "new physics" parameters such as $S$ [1201, 1202, a measure of possible new heavy chiral doublets such as a 4 th generation, or $m_{W^{*}}$, the scale of possible Kaluza-Klein excitations.

The most precise determinations of $\sin ^{2} \theta_{W}$ come from two measurements at SLAC [1203] and CERN 1204

$$
\begin{array}{ll}
\sin ^{2} \theta_{W}\left(m_{Z}\right)_{\overline{M S}} & =0.23070(26) \quad(\text { SLAC })  \tag{6.4}\\
\sin ^{2} \theta_{W}\left(m_{Z}\right)_{\overline{M S}} & =0.23193(29) \quad(\text { CERN }),
\end{array}
$$

with both extracting $\sin ^{2} \theta_{W}$ at the Z pole and carrying an error of roughly $0.1 \%$ level. Unfortunately, they disagree by about 3 sigma and therefore, individually provide completely different implications for the Higgs mass and possible "new physics". For example, the SLAC left-right asymmetry result weighs heavily in the leptonic Z pole average which indicates a Higgs mass of

$$
\begin{equation*}
m_{H} \approx 50_{-23}^{+34} \mathrm{GeV} \tag{6.5}
\end{equation*}
$$



Figure 6.1. The past, currently running, and future experiments on extracting $\sin ^{2} \theta_{W}(Q)$.
with the center value significantly below the LEP II direct search limit [3]

$$
\begin{equation*}
m_{H}>114 \mathrm{GeV}(95 \% \mathrm{C} . \mathrm{L} .) . \tag{6.6}
\end{equation*}
$$

On the other hand, the LEP $Z \rightarrow b \bar{b}$ forward-backward asymmetry weights heavily in the hadronic Z pole average which implies a rather heavy Higgs [1205]

$$
\begin{equation*}
m_{H} \approx 480_{-230}^{+350} \mathrm{GeV} \tag{6.7}
\end{equation*}
$$

The often quoted bound $m_{H}<150 \mathrm{GeV}$ results mainly from the Z-pole world average $\sin ^{2} \theta_{W}\left(m_{Z}\right)_{\overline{M S}}=0.23125(16)$. Is the world average correct? We may have to wait and see what the LHC tells us.

In addition to experiments at the Z pole, several precision measurements of $\sin ^{2} \theta_{W}$ have been carried out at lower $Q^{2}$, including atomic parity violation [1206], polarized Moller scattering [1207, and deep-inelastic neutrino scattering [1208], but with uncertainties about an order of magnitude larger, i.e. $\mathcal{O}(1 \%)$. Together all such measurements play an important role in constraining "new physics" appendages to the SM, such as heavy $Z$ ' bosons of $\mathcal{O}(1$ TeV ) and are useful for demonstrating the running of $\sin ^{2} \theta_{W}(Q)$, due to $\gamma-Z$ loop mixing, at about the 6 sigma level.

It is highly desirable to have other experimental extractions of $\sin ^{2} \theta_{W}$ with a precision roughly comparable to Z pole measurements, given the $3 \sigma$ discrepancy between the two best values. Fortunately, several new measurements are in progress or planned at Jefferson lab, including $Q_{\text {weak }}$ using elastic ep scattering [1209] ( $\pm 0.0008$ ), polarized Moller scattering [1210] ( $\pm 0.00025$ ), and SOLID using polarized ed-DIS ( $\pm 0.0006$ ), which aim to extract $\sin ^{2} \theta_{W}$ at low $Q^{2}$ in very high luminosity fixed target experiments. Their projected uncertainties are shown in figure 6.1.

Here, we focus on the feasibility of measuring $\sin ^{2} \theta_{W}$ at high $Q^{2}$ using an Electron-Ion Collider (EIC). Since the center of mass energy of the EIC is expected to be much higher than
fixed target experiments, parity violating asymmetries are larger and, therefore, potentially more sensitive to weak interaction effects. In addition, the EIC enables one to extract $\sin ^{2} \theta_{W}(Q)$ and demonstrate its evolution over a wide range of $Q^{2}$. Those measurements will test the predicted running of $\sin ^{2} \theta_{W}\left(Q^{2}\right)$, improve the world average $\sin ^{2} \theta_{W}\left(m_{Z}\right)_{\overline{M S}}$, and test for "new physics" such as $Z^{\prime}$ bosons via comparison with Z-pole and low $Q^{2}$ results. We demonstrate those capabilities for an EIC with integrated luminosity of $200 \mathrm{fb}^{-1}, \sqrt{s} \approx 140$ GeV and electron (as well as perhaps hadron) polarization. A statistical determination of $\sin ^{2} \theta_{W}\left(Q^{2}\right)$ to about $\pm 0.25 \%$ is found for a range of $Q^{2}$ with overall precision roughly equal to the best Z-pole and proposed polarized $e^{-} e^{-}$measurements.

### 6.2.2 Extracting $\sin ^{2} \theta_{W}$ from parity-violating right-left polarization asymmetries

Various parity violating asymmetries in $e p$ - and $e d$ (deuteron)-DIS can be obtained from ratios of differences and sums of cross-sections with opposite polarizations

$$
\begin{align*}
& d \bar{\sigma}\left(P_{e}, P_{p, d}\right)-d \bar{\sigma}\left(-P_{e},-P_{p, d}\right) \propto  \tag{6.8}\\
& \frac{1}{2} \Sigma_{i} f_{i}(x)\left\{\left(P_{e}+\tilde{f}_{i}(x) P_{p, d}\right)\left(d \sigma_{R R}^{i}-d \sigma_{L L}^{i}\right)\right. \\
& \left.\quad+\left(P_{e}-\tilde{f}_{i}(x) P_{p, d}\right)\left(d \sigma_{R L}^{i}-d \sigma_{L R}^{i}\right)\right\}
\end{align*}
$$

and

$$
\begin{align*}
& d \bar{\sigma}\left(P_{e}, P_{p, d}\right)+d \bar{\sigma}\left(-P_{e},-P_{p, d}\right) \propto  \tag{6.9}\\
& \frac{1}{2} \Sigma_{i} f_{i}(x)\left\{\left(1+\tilde{f}_{i}(x) P_{e} P_{p, d}\right)\left(d \sigma_{R R}^{i}+d \sigma_{L L}^{i}\right)\right. \\
& \left.\quad+\left(1-\tilde{f}_{i}(x) P_{e} P_{p, d}\right)\left(d \sigma_{R L}^{i}+d \sigma_{L R}^{i}\right)\right\}
\end{align*}
$$

where $P_{e}$ and $P_{p, d}$ are longitudinal polarizations of the electron and proton (deuteron) beams. The $\alpha$ and $\beta$ in $d \sigma_{\alpha \beta}^{i}(\alpha, \beta=R, L)$ label polarizations of the electron and quark of type $i$, respectively. The $f_{i}(x)$ is the unpolarized parton distribution function and

$$
\begin{equation*}
\tilde{f}_{i}(x) \equiv \Delta f_{i}(x) / f_{i}(x) \tag{6.10}
\end{equation*}
$$

is the ratio of polarized and unpolarized parton distribution function. The quantity $\tilde{f}_{i}(x) P_{p, d}$ can be viewed as the effective quark longitudinal polarization in a polarized proton (deuteron).

The polarized electron-quark cross-sections are proportional to 1211

$$
\begin{align*}
d \sigma_{R R}^{i} & \propto\left(\frac{Q_{R e}^{\gamma} Q_{R i}^{\gamma}}{Q^{2}}+\frac{Q_{R e}^{Z} Q_{R i}^{Z}}{Q^{2}+M_{Z}^{2}}\right)^{2} \\
d \sigma_{L L}^{i} & \propto\left(\frac{Q_{L e}^{\gamma} Q_{L i}^{\gamma}}{Q^{2}}+\frac{Q_{L e}^{Z} Q_{L i}^{Z}}{Q^{2}+M_{Z}^{2}}\right)^{2} \\
d \sigma_{R L}^{i} & \propto\left(\frac{Q_{R e}^{\gamma} Q_{L i}^{\gamma}}{Q^{2}}+\frac{Q_{R e}^{Z} Q_{L i}^{Z}}{Q^{2}+M_{Z}^{2}}\right)^{2}(1-y)^{2} \\
d \sigma_{L R}^{i} & \propto\left(\frac{Q_{L e}^{\gamma} Q_{R i}^{\gamma}}{Q^{2}}+\frac{Q_{L e}^{Z} Q_{R i}^{Z}}{Q^{2}+M_{Z}^{2}}\right)^{2}(1-y)^{2} \tag{6.11}
\end{align*}
$$

Left-handed and right-handed couplings of electrons and quarks to the photon are the same

$$
\begin{equation*}
Q_{L}^{\gamma}=Q_{R}^{\gamma} \equiv Q^{\gamma} \tag{6.12}
\end{equation*}
$$

while those to the $Z$ are different (giving rise to parity violation)

$$
\begin{align*}
Q_{L}^{Z} & =\frac{e}{\sin \theta_{W} \cos \theta_{W}}\left(T_{3 L}-Q^{\gamma} \sin ^{2} \theta_{W}\right) \\
Q_{R}^{Z} & =\frac{e}{\sin \theta_{W} \cos \theta_{W}}\left(-Q^{\gamma} \sin ^{2} \theta_{W}\right) \tag{6.13}
\end{align*}
$$

with

$$
\begin{align*}
& Q_{u}^{\gamma}=\frac{2}{3}, Q_{d}^{\gamma}=-\frac{1}{3}, Q_{e}^{\gamma}=-1, \\
& T_{3 L}^{u}=\frac{1}{2}, T_{3 L}^{d}=T_{3 L}^{e}=-\frac{1}{2} . \tag{6.14}
\end{align*}
$$

For an ep collider, there are two single-polarization parity violating right-left asymmetries

$$
\begin{align*}
A_{e p}^{e} & \equiv \frac{d \bar{\sigma}\left(P_{e}, P_{p}=0\right)-d \bar{\sigma}\left(-P_{e}, P_{p}=0\right)}{d \bar{\sigma}\left(P_{e}, P_{p}=0\right)+d \bar{\sigma}\left(-P_{e}, P_{p}=0\right)}  \tag{6.15}\\
& =P_{e} \frac{\Sigma_{i} f_{i}(x)\left[\left(d \sigma_{R R}^{i}-d \sigma_{L L}^{i}\right)+\left(d \sigma_{R L}^{i}-d \sigma_{L R}^{i}\right)\right]}{\Sigma_{i} f_{i}(x)\left[\left(d \sigma_{R R}^{i}+d \sigma_{L L}^{i}\right)+\left(d \sigma_{R L}^{i}+d \sigma_{L R}^{i}\right)\right]}
\end{align*}
$$

and

$$
\begin{align*}
A_{e p}^{p} & \equiv \frac{d \bar{\sigma}\left(P_{e}=0, P_{p}\right)-d \bar{\sigma}\left(P_{e}=0,-P_{p}\right)}{d \bar{\sigma}\left(P_{e}=0, P_{p}\right)+d \bar{\sigma}\left(P_{e}=0,-P_{p}\right)}  \tag{6.16}\\
& =P_{p} \frac{\Sigma_{i} \Delta f_{i}(x)\left[\left(d \sigma_{R R}^{i}-d \sigma_{L L}^{i}\right)-\left(d \sigma_{R L}^{i}-d \sigma_{L R}^{i}\right)\right]}{\sum_{i} f_{i}(x)\left[\left(d \sigma_{R R}^{i}+d \sigma_{L L}^{i}\right)+\left(d \sigma_{R L}^{i}+d \sigma_{L R}^{i}\right)\right]}
\end{align*}
$$

with electron and proton separately polarized.
These asymmetries are simplified for an ed collider since the deuteron is an iso-singlet. Restricting to the large $x$ region ( $x>0.2$ ), the anti-quark contributions can be neglected. To first approximation, the parton distributions of $u$ and $d$ quark are the same (up to charge symmetry violation effects) in the deuteron and can thus be factored out of the sum over quark flavors. They then cancel in the asymmetries

$$
\begin{align*}
\left.A_{e d}^{e}\right|_{x>0.2} & \equiv \frac{d \bar{\sigma}\left(P_{e}, P_{d}=0\right)-d \bar{\sigma}\left(-P_{e}, P_{d}=0\right)}{d \bar{\sigma}\left(P_{e}, P_{d}=0\right)+d \bar{\sigma}\left(-P_{e}, P_{d}=0\right)}  \tag{6.17}\\
& =P_{e} \frac{\Sigma_{i}\left[\left(d \sigma_{R R}^{i}-d \sigma_{L L}^{i}\right)+\left(d \sigma_{R L}^{i}-d \sigma_{L R}^{i}\right)\right]}{\sum_{i}\left[\left(d \sigma_{R R}^{i}+d \sigma_{L L}^{i}\right)+\left(d \sigma_{R L}^{i}+d \sigma_{L R}^{i}\right)\right]}
\end{align*}
$$

and

$$
\begin{align*}
\left.A_{e d}^{d}\right|_{x>0.2} & \equiv \frac{d \bar{\sigma}\left(P_{e}=0, P_{d}\right)-d \bar{\sigma}\left(P_{e}=0,-P_{d}\right)}{d \bar{\sigma}\left(P_{e}=0, P_{d}\right)+d \bar{\sigma}\left(P_{e}=0,-P_{d}\right)}  \tag{6.18}\\
& =\tilde{f}^{D} P_{d} \frac{\Sigma_{i}\left[\left(d \sigma_{R R}^{i}-d \sigma_{L L}^{i}\right)-\left(d \sigma_{R L}^{i}-d \sigma_{L R}^{i}\right)\right]}{\Sigma_{i}\left[\left(d \sigma_{R R}^{i}+d \sigma_{L L}^{i}\right)+\left(d \sigma_{R L}^{i}+d \sigma_{L R}^{i}\right)\right]} .
\end{align*}
$$



Figure 6.2. The right-left asymmetries $A_{e p}^{e}$ and $A_{e d}^{e}$ as functions of $Q$ for $e p$ - and $e d$ - DIS at $\sqrt{s}=140$ GeV with polarized electron $\left(P_{e}=0.8\right)$.

This leads to some simplification in the case of the single-polarization asymmetry $A_{e d}^{e}(x)$ for the $e d$ collider over $A_{e p}^{e}(x)$ for the $e p$ collider. Both $A_{e p}^{e}(x)$ and $A_{e d}^{e}(x)$ are proportional to electron polarization $P_{e}$ and thus carry smaller uncertainties than asymmetries $A_{e p}^{p}(x)$ and $A_{e d}^{d}(x)$ which are proportional to the hadron polarization $P_{p, d}$ which has a larger uncertainty. In fact, the single-polarization asymmetries $A_{e p}^{p}(x)$ and $A_{e d}^{d}(x)$ with a hadron beam polarized would hardly play any role for the purpose of measuring $\sin ^{2} \theta_{W}$ to high precision due to the large uncertainty in $P_{p, d}$ expected to be $\mathcal{O}( \pm 5 \%)$. Instead, hadron polarization (or quark polarization) may be precisely determined from the asymmetries.

The double-polarization asymmetries

$$
\begin{align*}
& A_{e p, e d}^{e p, e d} \equiv \frac{d \bar{\sigma}\left(P_{e}, P_{p, d}\right)-d \bar{\sigma}\left(-P_{e},-P_{p, d}\right)}{d \bar{\sigma}\left(P_{e}, P_{p, d}\right)+d \bar{\sigma}\left(-P_{e},-P_{p, d}\right)}  \tag{6.19}\\
= & \frac{\Sigma_{i} f_{i}(x)\left\{\left(P_{e}+\tilde{f}_{i}(x) P_{p, d}\right)\left(d \sigma_{R R}^{i}-d \sigma_{L L}^{i}\right)+\left(P_{e}-\tilde{f}_{i}(x) P_{p, d}\right)\left(d \sigma_{R L}^{i}-d \sigma_{L R}^{i}\right)\right\}}{\Sigma_{i} f_{i}(x)\left\{\left(1+\tilde{f}_{i}(x) P_{e} P_{p, d}\right)\left(d \sigma_{R R}^{i}+d \sigma_{L L}^{i}\right)+\left(1-\tilde{f}_{i}(x) P_{e} P_{p, d}\right)\left(d \sigma_{R L}^{i}+d \sigma_{L R}^{i}\right)\right\}}
\end{align*}
$$

for both $e p$ and ed collider running depend on hadron polarization; however, there are circumstances for which the asymmetry can be simplified and carry a reduced uncertainty. First, the $d \sigma_{R L, L R}$ are proportional to $(1-y)^{2}$ and thus suppressed in the kinematic region $y \rightarrow 1$. Second, the double-polarization asymmetry can be further simplified for a ed collider at large $x$. As a result, the asymmetry

$$
\begin{equation*}
\left.A_{e d}^{e d}\right|_{y \rightarrow 1, x>0.2} \approx P_{\text {eff. }} \frac{\Sigma_{i}\left(d \sigma_{R R}^{i}-d \sigma_{L L}^{i}\right)}{\Sigma_{i}\left(d \sigma_{R R}^{i}+d \sigma_{L L}^{i}\right)} \tag{6.20}
\end{equation*}
$$

is proportional to the effective polarization

$$
\begin{equation*}
P_{\text {eff. }} \equiv \frac{P_{e}+\tilde{f}(x) P_{d}}{1+\tilde{f}(x) P_{e} P_{d}} \tag{6.21}
\end{equation*}
$$

which carries a reduced fractional uncertainty.
From the above discussion, it is clear that with regard to precision $\sin ^{2} \theta_{W}$ measurements, the most useful asymmetries are the two single-polarization asymmetries $A_{e p}^{e}$ and $A_{e d}^{e}$ with only the electron polarized for $e p$ and $e d$ collisions, respectively, and the double-polarization


Figure 6.3. The figure of merit of measuring the asymmetries $A_{e p}^{e}$ and $A_{e d}^{e}$ at an $e p$ and $e d$ collider with $\sqrt{s}=140 \mathrm{GeV}$ and polarized electron $\left(P_{e}=0.8\right)$, integrated luminosity of $200 \mathrm{fb}^{-1}$, for bin size of 10 GeV . A cut of $x>0.2$ is imposed for ed collisions.
asymmetry $A_{e d}^{e d}$ for the $e d$ collision, since they carry the smallest systematic polarization errors.

In general, the high energy EIC gains some advantage over experiments at low energy. For example, the error from higher $1 / Q^{2}$ twist effects should be negligible at high $Q$. In addition, since the uncertainty from parton distributions largely cancel in $A_{e d}^{e}$, the major source of systematic error comes from the polarization of electron beam $P_{e}$ which is expected to carry an uncertainty of roughly $\pm 0.5 \%$. This leads to an uncertainty of $\pm 0.5 \%$ in the single-polarization asymmetries $A_{e p, e d}^{e}$ and roughly $\pm 0.25 \%$ in $\sin ^{2} \theta_{W}$. One possible way to obtain some leverage on extracting $\sin ^{2} \theta_{W}$ with further reduced systematic error is to make use of the $y$ dependence to extract the term proportional to the vector coupling $g_{V}^{e} \propto 1-4 \sin ^{2} \theta_{W}$ of electrons to the $Z$ boson. It is well known that this coupling is very sensitive to $\sin ^{2} \theta_{W}$. An accuracy of $1 \%$ of the asymmetry proportional to this coupling determines $\sin ^{2} \theta_{W}$ at the $0.1 \%$ level. This may help with the systematic precision but unlikely with the statistical one since the latter would decrease in extracting various pieces from the $y$ dependence. To assess the statistic error in measuring $\sin ^{2} \theta_{W}$, we carry out a Monte Carlo simulation for polarized ep- and ed- DIS at $\sqrt{s}=140 \mathrm{GeV}$ as an example. We use the parton distribution functions of CTEQ6L 82]. We have included $u$ and $d$ quark and anti-quark contributions. For ed-DIS, a cut of $x>0.2$ is imposed to suppress the anti-quark contribution as needed to simplify the asymmetry in equation 6.17. We show the asymmetries $A_{e p}^{e}$ and $A_{e d}^{e}$ for $e p$ and $e d$ collider with polarized electron $\left(P_{e}=0.8\right)$ in figure 6.2. The asymmetries grow with $Q$ and reach $14 \%$ and $17 \%$ for $Q \approx 70 \mathrm{GeV}$, for ep and ed collisions, respectively.

Based on these polarized cross-sections, one can further obtain the statistical figure of merit (F.O.M.) $A^{2} N /\left(1-A^{2}\right) \approx A^{2} N$ for measuring the asymmetry and the statistical errors for a given luminosity. In figure 6.3, we show the figure of merit for $e p$ and $e d$ collisions with integrated luminosity of $200 \mathrm{fb}^{-1}$ as function of $Q$, with bin size of 10 GeV .

The corresponding statistical errors, $\Delta A / A \approx\left(A^{2} N\right)^{-1 / 2}$, are shown in figure 6.4 for $e p$ and $e d$ colliders. For an ed collider, the energy of the deuteron beam is shared by the proton and neutron, thus effectively the CM energy for e-nucleon is reduced from 140 GeV to roughly 100 GeV . For both $e p$ and ed collider, with 10 GeV bin, the statistical error is about $\pm 0.5 \%$ for $Q$ between 10 and 50 GeV . For $Q>50$ and $Q<10 \mathrm{GeV}$ region, the statistical error is significantly higher. However, a smaller error is achievable for $Q>50$


Figure 6.4. The statistical error expected for the asymmetries $A_{e p}^{e}$ and $A_{e d}^{e}$ for $e p$ and $e d$ collider at $\sqrt{s}=140 \mathrm{GeV}$ with polarized electron $\left(P_{e}=0.8\right)$, and with luminosity of $200 \mathrm{fb}^{-1}$, for bin size of 10 GeV . A cut of $x>0.2$ is imposed for $e d$ collider. The statistical error for $\sin ^{2} \theta_{W}(Q)$ is roughly $1 / 2$ the percentage error on $A_{e p}^{e}$ or $A_{e d}^{e}$.

GeV region if a larger bin is used. Overall, the error in extracting $\sin ^{2} \theta_{W}$ is roughly half of the error in the asymmetry. Therefore, the statistical error in extracting $\sin ^{2} \theta_{W}$ for most of the $Q$ region between a few GeV and Z-pole is below $\pm 0.25 \%$ level.

### 6.2.3 Conclusions

The advantage of measuring $\sin ^{2} \theta_{W}$ at a polarized EIC lies in its high $Q^{2}$, which enhances the parity violating asymmetry, reduces some of the uncertainty from higher twist effects, and most importantly enables one to extract $\sin ^{2} \theta_{W}$ over a wide range of $Q$ from a few GeV to $Q \approx m_{Z}$. We demonstrated the capability of measuring $\sin ^{2} \theta_{W}$ for an EIC with integrated luminosity of $200 \mathrm{fb}^{-1}, \sqrt{s} \approx 140 \mathrm{GeV}$ and electron (as well as perhaps hadron) polarization. A statistical determination of $\sin ^{2} \theta_{W}\left(Q^{2}\right)$ to about $\pm 0.25 \%$ is found for most of the region of $Q$ with overall precision roughly equal to the best Z-pole measurements. In figure 6.1, we have plotted values of $\sin ^{2} \theta_{W}(Q)$ obtained from past, ongoing and planned as well a possible EIC measurements. The running of $\sin ^{2} \theta_{W}(Q)$ is based on ref. 1212, 1213. The error bar for EIC measurements only represents the statistical error based on figure 6.4. A combination of all the measurements of $\sin ^{2} \theta_{W}$ at various scales will play very important roles in revealing the physics behind EWSB and other "new physics".

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### 6.3 Electron-to-Tau conversion

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### 6.3.1 Introduction and Motivation

Every conservation law in the Standard Model (SM) is anticipated to have a symmetry associated with it. We have no knowledge of a symmetry that asserts Lepton Flavor Conservation in the Standard Model (SM) of particle physics and yet its (direct) violation has never been seen. Although discovery of neutrino oscillations [1214, 1215] indicates that charged Lepton Flavor Violation (LFV) processes such as $\mu \rightarrow e \gamma$ should be allowed (within the SM), its rate is expected to be very small $\left(\operatorname{BR}(\mu \rightarrow e \gamma)<10^{-54}\right)$ due to the very small values of the neutrino masses. This level of sensitivity is beyond the reach of any present or planned experiment. However, many models of physics Beyond the SM (BSM) predict rates of charged lepton flavor violation significantly higher than those within the SM, some of them even within the reach of present or planned experiments. LFV hence becomes a very attractive process for experimental discovery of physics beyond the Standard Model.

Many searches for specific reactions which violate lepton flavor have been performed. The most sensitive include searches for $\mu+N \rightarrow e+N$ using low energy muons (from the SINDRUM II collaboration [1216]), the muon decay $\mu \rightarrow e \gamma$ (MEGA collaboration [1217, [1218]), and decays of kaons ( 1219 ). The limits from these processes, though extremely precise, are all sensitive to $e \leftrightarrow \mu$ transitions (abbreviated $\operatorname{LFV}(1,2)$ ) and not to $e \leftrightarrow \tau$ transitions (LFV(1,3)). Also, each of these processes involve specific quark flavors: in some, only the 1st generation quarks participate; in others the same quark flavor must couple to the initial and final leptons, or strange quarks must participate. These stringent bounds are related to the opportunities for such searches afforded by specific experimental apparatuses. None of these searches involved the $\tau$ lepton either in the initial or in the final state. Since a general model with lepton flavor violation may involve a $\tau$ lepton and also initial and final state quarks of different flavors (not necessarily including strange quarks), the above measurements would be blind to such LFV mechanisms. Existing best limits on $e \leftrightarrow \tau$ conversion come from the BaBar Collaboration $(\tau \rightarrow e \gamma)$ 1220 and the BELLE Collaboration $(\tau \rightarrow 3 e)$ [1221. These are notably worse than the limits on $e \leftrightarrow \mu$ by several orders of magnitude. LFV searches at proposed future experiments would further improve limits on $e \leftrightarrow \mu$ transitions.

The search for LFV involving $\tau$ leptons has been performed by the high energy lepton - hadron collider experiments H1 and ZEUS. The LFV process could proceed via exchange of a leptoquark (LQ), a color triplet boson - scalar or vector - with both lepton and baryon quantum numbers which appears naturally in many extensions of the SM such as GUTs, supersymmetry, compositeness, and technicolor (for a concise review of LFV in several such models, see [1222]). The most recent limits on the search for $e p \rightarrow \mu X$ and $e p \rightarrow \tau X$ were set by the H1 collaboration using HERA collisions at 320 GeV center-of-mass energy and an integrated luminosity of $0.5 \mathrm{fb}^{-1}$. They did not find any evidence for lepton flavor violation [1223, 1224], and in turn they put limits on the mass and couplings of the leptoquarks in the Buchmüller-Rückl-Wyler (BRW) effective model 1225 .

A high energy, high luminosity electron-proton/ion collider (EIC) is being considered by the US nuclear science community with a variable center-of-mass energy of $50 \rightarrow 160$ GeV and with $100-1000$ times the accumulated luminosity of HERA over a comparable operation time, see sections 7.1 and 7.2 . In a recent study [1226] it has been argued that a

90 GeV center-of-mass e-p collider with $10 \mathrm{fb}^{-1}$ of integrated luminosity could set a limit on leptoquark coupling-over-mass ratios that would surpass the current best limits from HERA experiments. The study also shows that the proposed EIC could compete or surpass the updated leptoquark limits from $\tau \rightarrow e \gamma$ for a subset of quark flavor diagonal couplings. Lastly, the authors found that although $e \rightarrow \tau$ LFV is indeed severely suppressed, $e \rightarrow \tau$ transition could still exist within the reach of the EIC, under certain situations [1226]. The present study of search for leptoquarks at the EIC was motivated by these exciting possibilities.

For completeness, we studied leptoquark couplings with first, second and third generation leptons ( $e \rightarrow e, \mu, \tau$ ) in our simulations, although the main focus of this study was the $e \rightarrow \tau$ transition. We comment here on all three.

1. Leptoquark decays to first generation leptons lead to final states similar to those in SM deep inelastic scattering (DIS) neutral current (NC, ep $\rightarrow e X$ ) and charged current $(\mathrm{CC}, e p \rightarrow \nu X)$ interactions. These processes contribute as backgrounds by mimicking the final state signature of the signal events, and hence are indistinguishable. Other SM backgrounds arise from photo-production $\gamma p \rightarrow X$, lepton-pair production (ep $\rightarrow$ $e l^{+} l^{-} X$ ), and W production ( $e p \rightarrow e W X$ ). We simulate them and study the angular correlations of the final states and the missing momentum spectra in cases where neutrinos are involved in the final state. Possibilities of misidentification of events due to detector inefficiencies will be commented upon in section 6.3.7,
2. Leptoquark decays with a $\mu$ in the final state give a back-to-back muon and hadronic system event characteristic in the transverse plane. Since muons typically deposit a very small fraction of their energy in a calorimeter, in real experiments, such events are characterized by a large missing calorimetric transverse momentum. Additionally, such muons are typically required to be isolated, well separated from the hadronic jets or tracks in such an event. Such selections strongly suppress the NC component of the SM backgrounds, which mainly arise from muon-pair production and muonic decays of W bosons. See details in [1223, 1224].
3. The $1 \rightarrow 3$ transition, ep $\rightarrow \tau X$, is the principle focus of this study; it is studied using three $\tau$ decay channels: electronic, muonic and hadronic. Electronic decays $\tau \rightarrow e \nu_{e} \nu_{\tau}$ have a topology similar to high $Q^{2} \mathrm{NC}$ events, except for missing transverse momentum due to the escaping neutrinos, which can be exploited to reduce this background. Muonic decays $\tau \rightarrow \mu \nu_{\mu} \nu_{\tau}$ result in similar final states as the electronic decay of $\tau$ and hence a similar criteria for their selection is used. Hadronic decays of $\tau$ lead to a high transverse momentum, narrow jet resulting in a signal topology of a di-jet event with no leptons. These events can be selected using various well known algorithms to identify and separate the $\tau$-jet from other hadronic jets in NC DIS and photoproduction events.

Many of the above mentioned strategies require detailed detector simulation of the response. This is not done in the present study. However, we studied the event topologies of the SM processes and the leptoquark events through simulations with beam energies and detector acceptance guidelines suggested on the INT website [131. The differences in event topologies generated by $p_{T}^{\text {miss }}$ (the missing transverse momentum) and the angle $\phi$ (between the $\tau$-jet and the missing transverse momentum vector) present in SM and LQ events with final state neutrinos were studied. We ask in this study: are they different enough to be
distinguishable from one another at the EIC energies, and for what range of leptoquark couplings and masses could the LFV LQ events be differentiated from a SM event at the EIC.

This report proceeds as follows. In section 6.3.2, the leptoquark framework is introduced and the findings of [1226] are summarized and updated to reflect recent developments regarding higher EIC integrated luminosities and the proposed reach of Super-B experimental searches for $\tau \rightarrow e \gamma$. Section 6.3.3 discusses the possibility of $e \rightarrow \tau$ searches at the EIC in the broader context of an effective operator framework. Concluding remarks for the theoretical analysis are presented in section 6.3.4. An experimental analysis begins with section 6.3.5 in which we present the SM process generation and its study for the above correlations. In section 6.3.6 we detail the MC generator study for the leptoquark and study some of its parameters (leptoquark mass dependence and the coupling strength dependence) on the observable missing $p_{T}$ and $\phi$ spectra. In section 6.3.7 we compare some of the selected spectra from SM and the leptoquark and show potentially how leptoquarks may be identified at a future EIC. We then conclude with a comment on the limitations of this study and a brief plan for the near future.

### 6.3.2 Theory I: Leptoquark Framework

We begin our study of $e \rightarrow \tau$ conversion at the EIC by assuming a leptoquark framework. Leptoquarks (abbreviated LQs) are particles coupling to leptons and quarks which arise in models such as Pati-Salam color- $S U(4)$ and $S U(5)$ GUTs. Leptoquarks provide a useful framework for an initial analysis of $e \rightarrow \tau$ conversion because they allow for the conversion process to occur at tree level, as described further below, and so larger cross sections may be expected relative to other models which induce LFV through loop effects. Additionally, searches for leptoquark-induced $e \rightarrow \tau$ were performed at HERA, and so direct comparisons can be made between limits from HERA and potential limits from the EIC.

The class of particles which may be described as "leptoquarks" have a variety of properties: spin 0 or 1 ; fermion number $F=3 B+L=0$ or $\pm 2 ; S U(2)_{L}$ singlet, doublet, or triplet representations; and chiral couplings to $L$ - or $R$-handed leptons. We use the Buchmüller-Rückl-Wyler (BRW) parameterization of LQs 1225. In this parameterization, there are 14 different LQs encompassing all allowed combinations of the listed properties; their interactions with quarks and leptons are given by the renormalizable SM gauge-invariant Lagrangian in equation (6.22).

$$
\begin{align*}
\mathcal{L}_{L Q}= & \mathcal{L}_{F=0}+\mathcal{L}_{|F|=2} \\
\mathcal{L}_{F=0}= & h_{1 / 2}^{L} \bar{u}_{R} \ell_{L} S_{1 / 2}^{L}+h_{1 / 2}^{R} \bar{q}_{L} \epsilon e_{R} S_{1 / 2}^{R}+\tilde{h}_{1 / 2}^{L} \bar{d}_{R} \ell_{L} \tilde{S}_{1 / 2}^{L} \\
& \quad+h_{0}^{L} \bar{q}_{L} \gamma_{\mu} \ell_{L} V_{0}^{L^{\mu}}+h_{0}^{R} \bar{d}_{R} \gamma_{\mu} e_{R} V_{0}^{R \mu}+\tilde{h}_{0}^{R} \bar{u}_{R} \gamma_{\mu} e_{R} \tilde{V}_{0}^{R \mu} \\
& \quad+h_{1}^{L} \bar{q}_{L} \gamma_{\mu} \vec{\tau} \ell_{L} \vec{V}_{1}^{L \mu}+\text { h.c. }  \tag{6.22}\\
\mathcal{L}_{|F|=2}= & g_{0}^{L} \bar{q}_{L}^{c} \epsilon \ell_{L} S_{0}^{L}+g_{0}^{R} \bar{u}_{R}^{c} e_{R} S_{0}^{R}+\tilde{g}_{0}^{R} \bar{d}_{R}^{c} e_{R} \tilde{S}_{0}^{R}+g_{1}^{L} \bar{q}_{L}^{c} \epsilon \vec{\tau} \ell_{L} \vec{S}_{1}^{L} \\
& \quad+g_{1 / 2}^{L} \bar{d}_{R}^{c} \gamma_{\mu} \ell_{L} V_{1 / 2}^{L \mu}+g_{1 / 2}^{R} \bar{q}_{L}^{c} \gamma_{\mu} e_{R} V_{1 / 2}^{R \mu} \\
& \quad+\tilde{g}_{1 / 2}^{L} \bar{u}_{R}^{c} \gamma_{\mu} \ell_{L} \tilde{V}_{1 / 2}^{L \mu}+\text { h.c. }
\end{align*}
$$

In equation (6.22), $q_{L}$ and $\ell_{L}$ are the $S U(2)_{L}$ doublet quarks and leptons, $u_{R}, d_{R}, e_{R}$ are the $S U(2)_{L}$ singlet quarks and charged lepton, $\epsilon$ is the $S U(2)_{L}$ antisymmetric tensor $\left(\epsilon_{12}=-\epsilon_{21}=+1\right), \vec{\tau}=\left(\tau_{1}, \tau_{2}, \tau_{3}\right)$ are the Pauli matrices, and the charge conjugated fermion
is defined as $\psi^{c} \equiv C \bar{\psi}^{T}=i \gamma_{2} \gamma_{0} \bar{\psi}^{T}$ in the Dirac basis for the $\gamma$ matrices. Color, $S U(2)_{L}$, and flavor (generation) indices have been suppressed. We follow the notation used in the recent literature where spin-0 leptoquarks are $S$ and spin-1 are $V$, the subscript indicates the $S U(2)_{L}$ quantum number ( 0 for a singlet, $1 / 2$ for a doublet, 1 for a triplet), the superscript $L, R$ indicates the chirality of the lepton coupling to the leptoquark, and a tilde ( ${ }^{( }$) is used to distinguish between leptoquarks which have different hypercharges but are otherwise identical. The dimensionless coupling constants $g$ and $h$ (which we assume to be real) carry the same lepton chirality and $S U(2)_{L}$ labels as their associated leptoquarks. Lepton flavor violating processes mediated by LQs arise if the couplings - which are matrices in flavor space - have non-zero off-diagonal elements.

The $e \rightarrow \tau$ conversion process mediated by LQs is shown at the partonic level in the Feynman diagrams in figure 6.5. For simplicity, the couplings $g$ and $h$ in equation (6.22) have been replaced by $\lambda_{i j}$ where the first index corresponds to the lepton generation and the second index the quark generation. The cross section for the deep inelastic scattering conversion process $e^{-}+p \rightarrow \tau^{-}+X$ mediated by a single leptoquark is calculated using the Feynman rules derived from the Lagrangian of equation (6.22) and convoluting the partonic subprocess with the appropriate parton distribution functions for the initial state quark or antiquark. In the high mass approximation, where the LQ mass is much larger than the center-of-mass energy and all fermion masses are neglected, the momentum dependence of the LQ propagator can be neglected, effectively shrinking the propagator to a four fermion contact interaction. The cross section is then given by [1227]

$$
\begin{align*}
\sigma_{F=0}= & \sum_{\alpha, \beta} \frac{s}{32 \pi}\left[\frac{\lambda_{1 \alpha} \lambda_{3 \beta}}{M_{L Q}^{2}}\right]^{2}\left\{\int d x d y x \bar{q}_{\alpha}(x, x s) f(y)\right. \\
& \left.+\int d x d y x q_{\beta}(x,-u) g(y)\right\}, \\
\sigma_{|F|=2}=\sum_{\alpha, \beta} \frac{s}{32 \pi} & {\left[\frac{\lambda_{1 \alpha} \lambda_{3 \beta}}{M_{L Q}^{2}}\right]^{2}\left\{\int d x d y x q_{\alpha}(x, x s) f(y)\right.}  \tag{6.23}\\
& \left.+\int d x d y x \bar{q}_{\beta}(x,-u) g(y)\right\} .
\end{align*}
$$

The functions $f$ and $g$ are defined differently for scalar and vector leptoquarks:

$$
f(y)=\left\{\begin{array}{cc}
1 / 2 & (\text { scalar })  \tag{6.24}\\
2(1-y)^{2} & (\text { vector })
\end{array} \quad, g(y)=\left\{\begin{array}{cc}
(1-y)^{2} / 2 & \text { (scalar) } \\
2 & \text { (vector) }
\end{array} .\right.\right.
$$

The parton distribution functions for the quarks and antiquarks are $q\left(x, Q^{2}\right)$ and $\bar{q}\left(x, Q^{2}\right)$, respectively, evaluated at momentum fraction $x$ and energy scale $Q^{2}$. Also, $u=x s(y-1)$ and both $x$ and $y$ are integrated from 0 to 1 . As equation (6.23) shows, in the high mass approximation the unknown leptoquark couplings and masses appear in the cross section as the ratio $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$.

In the $e^{ \pm} p$ collisions at HERA, no $e \rightarrow \tau$ conversion events were observed. Limits on the LQ ratios $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ were set by both the ZEUS [1228] and H1 [1224] collaborations. In our analysis, we determine how the EIC might improve on these limits set by ZEUS and H1 by answering the question, to what values of the ratios $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ would the EIC be sensitive? As with the ZEUS and H1 analyses, we consider all combinations of the quark


Figure 6.5. Feynman diagrams showing the leptoquark-mediated $e \rightarrow \tau$ conversion process. $\alpha$ and $\beta$ are the quark generation indices.
generations $\alpha$ and $\beta$ (excluding the top quark) for all 14 BRW leptoquarks. It is assumed that one of the BRW LQs dominates the cross section and the LQs in $S U(2)_{L}$ multiplets are degenerate in mass. Full results of this analysis can be found in [1226]; in this report, we summarize the results and discuss a few representative examples.

With $1000 \mathrm{fb}^{-1}$ of integrated luminosity (attainable within a reasonable length of time at a high luminosity machine such as the EIC), the EIC would in principle be sensitive to $e \rightarrow \tau$ conversion cross sections at a level of 0.001 fb 1 This would yield on the order of one $e \rightarrow \tau$ conversion events (not accounting for backgrounds, $\tau$ reconstruction efficiency, etc.). Using this number for the cross section, and assuming a center-of-mass energy $\sqrt{s}=90 \mathrm{GeV}$, the LQ ratios $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ can be calculated from equation (6.23). Generally, for nearly all leptoquarks and combinations of quark generations $\alpha$ and $\beta$, the EIC could probe values of the ratios $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ that are smaller than the HERA limits by a factor between 10 and 200. This is demonstrated for the LQ $S_{0}^{R}$ in figures 6.6 and 6.7 where the cross sections for the different quark generation combinations $(\alpha \beta)$ are plotted as a function of the number $z$, defined to be the LQ ratio $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ scaled by the corresponding HERA limit. For example, the cross section for first generation initial and final state quarks (the red line in figure (6.6) is equal to 0.001 fb at $z \simeq 0.05$. This means that the EIC could improve the HERA limit on the ratio $\lambda_{11} \lambda_{31} / M_{L Q}^{2}$ for the leptoquark $S_{0}^{R}$ by as much as a factor of 20 ; or, if such a leptoquark exists and has properties such that $\lambda_{11} \lambda_{31} / M_{L Q}^{2}$ is between 0.05 and 1 times the HERA limit, this LQ could induce a number of $e \rightarrow \tau$ conversion events sufficiently large enough to be observed at the EIC.

Also shown in figure 6.6 are the values of the LQ ratios $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ (again scaled by the HERA limits) to which future Super-B experiments may be sensitive ${ }^{2}$; these are indicated

[^283]

Figure 6.6. The $e \rightarrow \tau$ cross section for the leptoquark $S_{0}^{R}$ plotted as a function of $z$, defined to be the ratio $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ scaled by the HERA limit. A cross section of 0.001 fb , corresponding to order 1 events with $1000 \mathrm{fb}^{-1}$ integrated luminosity, is indicated with a gray dashed line. The cross section is plotted for the different quark generation combinations, $(\alpha \beta)$. Shown here are the quark flavor-diagonal contributions with $\alpha=\beta$. The vertical dashed lines indicate the range of these ratios to which the Super-B experiments may be maximally sensitive from $\tau \rightarrow e \gamma$ searches.


Figure 6.7. As for figure 6.6] but shown here are the quark flavor-off-diagonal contributions with $\alpha \neq \beta$. No $\tau \rightarrow e \gamma$ limits exist in this case.


Figure 6.8. Feynman diagrams showing the leptoquark loops contributing to the $\tau \rightarrow e \gamma^{*}$ process.
with vertical dashed lines in the figure. The scalar leptoquarks can contribute to the $\tau \rightarrow e \gamma$ decay through loop diagrams shown in figure $\left[6.83^{3}\right.$ Limits on the LQ ratios are derived as follows. The amplitude for the process $\tau \rightarrow e \gamma^{*}$ has the general form [1229]

$$
\begin{align*}
& \mathcal{M}_{\tau \rightarrow e \gamma^{*}}=e \epsilon^{* \nu} \bar{u}_{e}\left(p^{\prime}\right)\left[\left(q^{2} \gamma_{\nu}-q_{\nu}(q \cdot \gamma)\right)\left(A_{1}^{L} P_{L}+A_{1}^{R} P_{R}\right)\right. \\
&\left.+i m_{\tau} q^{\alpha} \sigma_{\nu \alpha}\left(A_{2}^{L} P_{L}+A_{2}^{R} P_{R}\right)\right] u_{\tau}(p), \tag{6.25}
\end{align*}
$$

where the $A_{1} \mathrm{~s}$ and $A_{2}$ s are model-dependent factors. For a real photon, $q^{2}=0$, and so $|\mathcal{M}|^{2}$ depends only on the factors $A_{2}^{L, R}$. Then, the $\tau$ decay rate ratio is given by

$$
\begin{equation*}
R(\tau \rightarrow e \gamma) \equiv \frac{\Gamma\left(\tau^{-} \rightarrow e^{-} \gamma\right)}{\Gamma\left(\tau^{-} \rightarrow e^{-} \bar{\nu}_{e} \nu_{\tau}\right)}=\frac{48 \pi^{3} \alpha_{E M}}{G_{\mu}^{2}}\left(\left|A_{2}^{L}\right|^{2}+\left|A_{2}^{R}\right|^{2}\right) . \tag{6.26}
\end{equation*}
$$

Recent work by the BABAR collaboration [1220] has set a $90 \%$ C.L. limit $\Gamma(\tau \rightarrow e \gamma) / \Gamma_{\text {total }} \leq$ $3.3 \times 10^{-8}$. The current consensus is that future Super-B experiments will be able to improve this limit by a single order of magnitude, and so we take $R \leq 1.85 \times 10^{-8}$. The coefficients $A_{2}^{L}$ and $A_{2}^{R}$ can be determined for each scalar leptoquark by computing the amplitude for the $\tau \rightarrow e \gamma$ loop diagrams and picking out terms proportional to the magnetic moment operator $q^{\alpha} \sigma_{\nu \alpha}$. When neglecting the lepton masses and expanding in powers of $m_{q}^{2} / M_{L Q}^{2}$, at zeroth order the $A_{2}$ s will depend on a sum over $\alpha$ of the ratios $\lambda_{1 \alpha} \lambda_{3 \alpha} / M_{L Q}^{2}$ (here, $\alpha=\beta$ since there is only one quark present in the loop). Thus, the experimental limit on $R$ determines a range of upper limits on the LQ ratios: the stronger upper limit is set by assuming all three quark generations contribute to the $A_{2}$ coefficients equally, while the weaker upper limit assumes only a single quark generation contributes to the $A_{2}$ coefficients. Both upper limits on $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ (again scaled by the HERA limit) are indicated by vertical dashed lines for each quark generation in figure 6.6.

As figure 6.6 shows for the $S_{0}^{R}$ LQ, the EIC could potentially surpass upper limits on the LQ ratios derived from an improved Super-B factory $\tau \rightarrow$ er limit. For the other scalar leptoquarks, it is generally true that the EIC would be competitive with or surpass the future limits from Super-B factories. The EIC also has two additional advantages over $\tau \rightarrow e \gamma$ searches. First, $\tau \rightarrow e \gamma$ only constrains those leptoquark ratios $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$ for which $\alpha=\beta$, while the EIC can probe all combinations of quark generations. Second, it is possible for the LQ-induced $\tau \rightarrow e \gamma$ to be suppressed relative to $e \rightarrow \tau$ conversion: the first non-zero contribution to the $A_{2}$ coefficient may be proportional to $m_{q}^{2} / M_{L Q}^{2} \ll 1$ because of a cancellation of electric charges in the zeroth order term. Under these circumstances, the $\tau \rightarrow e \gamma$ yields relatively weak upper bounds on the LQ ratios. This occurs for the scalar leptoquark $\tilde{S}_{1 / 2}^{L}$.

Finally, we discuss the impact of $\operatorname{LFV}(1,2)$ searches on the leptoquark limits. As in the case of the effective operators below, a priori there is nothing in the BRW leptoquark parameterization that relates the LQ couplings to second generation leptons to LQ couplings to third generation leptons. Therefore, experimental limits on $\mu \rightarrow e$ conversion, $\mu \rightarrow e \gamma$, and $\mu \rightarrow 3 e$ do not necessarily affect the expected size of the cross sections expected for leptoquark-mediated $e \rightarrow \tau$ conversion at the EIC. Only by considering a specific model with an additional symmetry does a connection between LQ-induced $\operatorname{LFV}(1,2)$ and $\operatorname{LFV}(1,3)$ exist. An example is the $S U(5)$ GUT studied in [1230, 1231]. The leptoquark present in this model has the same spin and gauge group quantum numbers as the BRW leptoquark $\tilde{S}_{1 / 2}^{L}$.

[^284]

Figure 6.9. Feynman diagrams showing the contributions of the magnetic moment $\left(\mathcal{O}_{\sigma L, R}\right)$, four lepton $\left(\mathcal{O}_{\ell L, R}\right)$, and four fermion $\left(\mathcal{O}_{\ell q}\right)$ operators to the $e \rightarrow \tau$ conversion process.

As mentioned above, this particular LQ evades limits from $\tau \rightarrow e \gamma$ as well as $\mu \rightarrow e \gamma$ for the same reason. Additionally, the $S U(5)$ symmetry implies that the leptoquark couplings are proportional to the neutrino mixing angles and squared mass differences, and the stringent experimental bounds on $\mu \rightarrow e$ conversion further constrain the LQ couplings. Imposing all of these limits, the LQ couplings can still yield an $e \rightarrow \tau$ conversion cross section within reach of the EIC with $1000 \mathrm{fb}^{-1}$ integrated luminosity (for details, see [1231, [1226]). In particular, the $e^{-}+p \rightarrow \tau^{-}+X$ cross section is dominated by the partonic subprocess $e+d \rightarrow \tau+b$, implying that a $\tau$ plus a $b$-jet may be a unique experimental signatature of this particular $S U(5)$ GUT at the EIC.

### 6.3.3 Theory II: Effective Operators

We now examine the $e \rightarrow \tau$ conversion process at the EIC from the perspective of model-independent effective operators. A complete list of $S U(3)_{C} \times S U(2)_{L} \times U(1)_{Y}$ gaugeinvariant dimension- 5 and -6 operators built from the SM field content can be found in [1232] (for an updated list, see [1233]). There are three classes of operators which can contribute to $e \rightarrow \tau$ conversion and are of particular interest [1234, 1235]:

1. magnetic moment operators (written here after electroweak symmetry breaking)

$$
\begin{equation*}
\mathcal{O}_{\sigma L}=i m_{j} \bar{\ell}_{L i} \sigma^{\mu \nu} \ell_{R j} F_{\mu \nu}+\text { h.c. } ; \tag{6.27}
\end{equation*}
$$

2. four lepton operators

$$
\begin{equation*}
\mathcal{O}_{\ell L}=\bar{\ell}_{L i} \ell_{L j}^{C} \bar{\ell}_{L k}^{C} \ell_{L m} ; \tag{6.28}
\end{equation*}
$$

3. four fermion (two quark, two lepton) operators

$$
\begin{equation*}
\mathcal{O}_{\ell q}=\bar{\ell}_{i} \Gamma_{\ell} \ell_{j} \bar{q} \Gamma_{q} q \tag{6.29}
\end{equation*}
$$

We use indices $i, j, k, l$ to indicate the lepton generations and suppress the gauge group indices; the superscript ${ }^{C}$ indicates charge conjugation. Note that analogous operators with right-handed fields can also be constructed. These operators can contribute to the deep inelastic electron-to-tau conversion process, as shown in figure 6.9,

The leptonic current for the photon exchange diagrams in figure 6.9 (left and middle) has a general parameterization similar to the $\tau \rightarrow e \gamma$ amplitude in equation (6.25):

$$
\begin{align*}
j^{\mu}= & \bar{u}_{e}\left[\left(q^{2} \gamma^{\mu}-q^{\mu}(q \cdot \gamma)\right)\left(A_{1}^{L} P_{L}+A_{1}^{R} P_{R}\right)\right.  \tag{6.30}\\
& \left.+i m_{\tau} q_{\nu} \sigma^{\mu \nu}\left(A_{2}^{L} P_{L}+A_{2}^{R} P_{R}\right)\right] u_{\tau}
\end{align*}
$$

| $\tau \rightarrow 3 e$ | $\Gamma\left(\tau^{-} \rightarrow e^{-} e^{+} e^{-}\right) / \Gamma_{\text {total }}<3.6 \times 10^{-8}$ |
| :--- | :--- |
| $\tau \rightarrow e \mu \mu$ | $\Gamma\left(\tau^{-} \rightarrow e^{-} \mu^{+} \mu^{-}\right) / \Gamma_{\text {total }}<3.7 \times 10^{-8}$ |
| $\tau \rightarrow \mu e e$ | $\Gamma\left(\tau^{-} \rightarrow \mu^{-} e^{+} e^{-}\right) / \Gamma_{\text {total }}<2.7 \times 10^{-8}$ |
| $\tau \rightarrow 3 \mu$ | $\Gamma\left(\tau^{-} \rightarrow \mu^{-} \mu^{+} \mu^{-}\right) / \Gamma_{\text {total }}<3.2 \times 10^{-8}$ |
| $\tau \rightarrow e \gamma$ | $\Gamma\left(\tau^{-} \rightarrow e^{-} \gamma\right) / \Gamma_{\text {total }}<3.3 \times 10^{-8}$ |
| $\tau \rightarrow \mu \gamma$ | $\Gamma\left(\tau^{-} \rightarrow \mu^{-} \gamma\right) / \Gamma_{\text {total }}<4.4 \times 10^{-8}$ |

Table 6.2. All limits are taken from [3] and are at a $90 \%$ C.L.
The two structures in this current are the charge radius term, $q^{2} \gamma^{\mu}-q^{\mu}(q \cdot \gamma)$, with $A_{1}^{L, R}$ coefficients, and the magnetic moment term, $i m_{\tau} q_{\nu} \sigma^{\mu \nu}$, with $A_{2}^{L, R}$ coefficients. The loop diagram (middle) in figure 6.9 which contains the four fermion and four lepton operators contributes to the charge radius term of the leptonic current, and so the Wilson coefficients of the operators $\mathcal{O}_{\ell L, R}$ and $\mathcal{O}_{\ell q}$ appear in the coefficients $A_{1}^{L, R}$. These contributions are loop-suppressed but receive potentially large logarithmic enhancements which go like $\ln \left(\Lambda_{L F V}^{2} / m^{2}\right)$ (where $m$ is the mass of the quark or lepton in the loop and $\Lambda_{L F V}$ is the scale at which new degrees of freedom that induce LFV are no longer integrated out of the theory) [1234. The left photon exchange diagram in figure 6.9 containing the magnetic moment operator implies that the $A_{2}^{L, R}$ factors in the leptonic current depend on the Wilson coefficients of the $\mathcal{O}_{\sigma L, R}$ operators. These effective operators also are loop suppressed since they appear in the effective theory when heavy particles in loop diagrams (e.g., the leptoquarks in figure (6.8) are integrated out of the full theory.

The four fermion operator in figure 6.9 (right), similar to the Fermi theory for weak interactions, is a contact interaction that arises when a massive propagator is integrated out of the full theory at external momentum scales much smaller than the propagator's mass. This operator contributes to $e \rightarrow \tau$ conversion at tree level. Its cross section is expected to be larger than the cross sections from the other diagrams and operators discussed above (assuming the Wilson coefficients for all of the operators in equations (6.27)-(6.29) are all roughly the same order).

Limits on the magnetic moment and four lepton operator coefficients can be determined directly from relevant $\tau$ decay limits, some of which are listed in table 6.2, The smallness of the limits on these $\tau$ decays, in conjunction with loop suppression factors, ensures that the contributions of the $\mathcal{O}_{\sigma L, R}, \mathcal{O}_{\ell L, R}$ coefficients to the leptonic current in equation (6.30) are negligible. Therefore, as stated previously, it is expected that the greatest contributions to $e \rightarrow \tau$ conversion will come from the four fermion operators $\mathcal{O}_{\ell q}$, while photon exchange contributions will be negligibly small. Limits on the four fermion operators' coefficients can be determined from the limits on the leptoquark ratios $\lambda_{1 \alpha} \lambda_{3 \beta} / M_{L Q}^{2}$. The 14 leptoquarks in the BRW parameterization correspond to 7 of the four fermion operators listed in [1232], as shown in table 6.3 (though the correspondence is not one-to-one). Hence the leptoquark limits set by direct $e \rightarrow \tau$ searches at HERA as well as the rare process searches cited by the HERA analyses [1228, such as $\tau \rightarrow \pi e$ and decays of $B$ and $K$ mesons, allow limits to be set on the four fermion operator coefficients.

We conclude our discussion of the effective operators by noting that searches for $\mu \rightarrow e$ conversion, $\mu \rightarrow e \gamma$, and $\mu \rightarrow 3 e$ bound the coefficients of the operators in (6.27)-(6.29) which mix first and second generation leptons. However, a priori, limits on such LFV(1,2)

| $\mathcal{O}_{\ell q}^{(1)}$ | $\bar{\ell}_{L} \gamma_{\mu} \ell_{L} \bar{q}_{L} \gamma^{\mu} q_{L}$ | $\left(S_{0}^{L}, \vec{S}_{1}^{L}\right) ;\left(V_{0}^{L}, \vec{V}_{1}^{L}\right)$ |
| :--- | :--- | :--- |
| $\mathcal{O}_{\ell q}^{(3)}$ | $\bar{\ell}_{L} \gamma_{\mu} \tau^{a} \ell_{L} \bar{q}_{L} \gamma^{\mu} \tau^{a} q_{L}$ | $\left(S_{0}^{L}, \vec{S}_{1}^{L}\right) ;\left(V_{0}^{L}, \vec{V}_{1}^{L}\right)$ |
| $\mathcal{O}_{e u}$ | $\bar{e}_{R} \gamma_{\mu} e_{R} \bar{u}_{R} \gamma^{\mu} u_{R}$ | $S_{0}^{R} ; \tilde{V}_{0}^{R}$ |
| $\mathcal{O}_{e d}$ | $\bar{e}_{R} \gamma_{\mu} e_{R} \bar{d}_{R} \gamma^{\mu} d_{R}$ | $\tilde{S}_{0}^{R} ; V_{0}^{R}$ |
| $\mathcal{O}_{\ell u}$ | $\bar{\ell}_{L} u_{R} \bar{u}_{R} \ell_{L}$ | $S_{1 / 2}^{L} ; \tilde{V}_{1 / 2}^{L}$ |
| $\mathcal{O}_{\ell d}$ | $\bar{\ell}_{L} d_{R} \bar{d}_{R} \ell_{L}$ | $\tilde{S}_{1 / 2}^{L} ; V_{1 / 2}^{L}$ |
| $\mathcal{O}_{q e}$ | $\bar{q}_{L} e_{R} \bar{e}_{R} q_{L}$ | $S_{1 / 2}^{R} ; V_{1 / 2}^{R}$ |
| $\mathcal{O}_{q d e}$ | $\bar{\ell}_{L} e_{R} \bar{d}_{R} q_{L}$ |  |
| $\mathcal{O}_{\ell q}$ | $\bar{\ell}_{L} e_{R} \epsilon \bar{q}_{L} u_{R}$ |  |

Table 6.3. List of four fermion operators. For the operator names, we follow the notation of 1232 . In the middle column, we maintain the same notation as in equation (6.22). The right column lists the leptoquarks from which these operators are obtained upon integrating out the LQs. Some operators are a linear combination of different LQs which are enclosed in parentheses.
operators do not constrain the $\operatorname{LFV}(1,3)$ operators relevant for $e \rightarrow \tau$ conversion. Only by assuming the existence of an additional symmetry or a particular underlying model can the two sets of operators be related. One example of such an additional symmetry is the theory of minimal flavor violation (MFV) in the lepton sector [1236]. Under the assumptions of MFV, the breaking of the lepton flavor symmetry group $S U(3)_{L} \times S U(3)_{E}$ (for the left-handed doublets and the right-handed charged leptons) arises solely from the charged lepton and neutrino mass matrices 4 As a result, all higher-dimensional lepton flavor violating operators constructed from the lepton bilinears $\bar{\ell}_{L}^{i} \Gamma \ell_{L}^{j}, \bar{e}_{R}^{i} \Gamma \ell_{L}^{j}$, and $\bar{e}_{R}^{i} \Gamma e_{R}^{j}$ are suppressed by one or more powers of lepton masses and/or neutrino mixing parameters. This is true even of the four fermion type operators. Under the MFV hypothesis, the $e \rightarrow \tau$ conversion cross section is unobservably small; it is probable that any observation of $e \rightarrow \tau$ conversion at the EIC would therefore rule out the MFV hypothesis.

### 6.3.4 Theory III: Conclusions and Future Work

The theoretical analysis of the $e \rightarrow \tau$ DIS process presented in 1226 and section 6.3.2 shows that leptoquarks provide a framework in which $e \rightarrow \tau$ conversion searches at the EIC are feasible. Present leptoquark limits are not prohibitive, and the EIC would be competitive with future Super-B experiments ( $\tau \rightarrow e \gamma$ searches) on similar time scales, for several reasons: the EIC would have high luminosity and be sensitive to small cross sections; the EIC like HERA can set limits for all combinations of quark generations while $\tau \rightarrow e \gamma$ is more limited in this region; and the EIC could probe leptoquarks which may evade $\tau \rightarrow e \gamma$ searches.

Limits from $\operatorname{LFV}(1,2)$ searches may or may not be relevant for leptoquarks. While the BRW framework implies no connection between $\operatorname{LFV}(1,2)$ limits and $\operatorname{LFV}(1,3)$ processes, in general it is presumed that leptoquarks will arise from physics at the high scale which does in fact constrain $\operatorname{LFV}(1,3)$ processes given the current stronger limits on $\operatorname{LFV}(1,2)$ processes. However, at least one model, the $S U(5)$ GUT discussed above, exists in which

[^285]limits from $\operatorname{LFV}(1,2)$ searches $(\mu \rightarrow e$ conversion, $\mu \rightarrow e \gamma), \tau \rightarrow e \gamma$ searches, and the neutrino sector can be implemented and still allow for observable $e \rightarrow \tau$ conversion cross sections at the EIC.

An estimation of $e \rightarrow \tau$ cross sections using model-independent effective operators and present limits on $L F V$ processes suggests that the best hope for observing $e \rightarrow \tau$ conversion at the EIC is with models which give rise to four fermion operators through tree level processes at low energies. Four lepton and magnetic moment operators are generally too suppressed to give rise to large enough $e \rightarrow \tau$ cross sections via photon exchange, especially when the relevant limits (e.g., $\tau \rightarrow 3 e, \tau \rightarrow e \gamma$ ) are imposed on the operator coefficients. Limits from additional LFV $(1,2)$ searches like $\mu \rightarrow e$ conversion and $\mu \rightarrow e \gamma$ can be applied to the effective operator analysis if an additional symmetry such as MFV is imposed. MFV results in a suppression of all the LFV operators, including the four fermion operators, and hence negligibly small $e \rightarrow \tau$ cross sections.

There are several theoretical topics worthy of further attention for the $e \rightarrow \tau$ EIC search. First is the study of leptoquarks and $\operatorname{LFV}(1,3)$ flavor structure at LHC. While studies of LQ searches at the LHC have been performed in the past (as an example, see [1237]), such work has focused only on first generation fermions coupling to leptoquarks and has not considered LFV leptoquark final states. Further work is required to determine the extent to which the EIC and the LHC may provide complementary probes of the leptoquark flavor violating parameter space.

An additional topic which merits further study is a broader analysis of model-dependent $e \rightarrow \tau$ searches at the EIC. Non-leptoquark models or symmetries may give promising results for the $e \rightarrow \tau$ conversion process. For example, R-parity violating supersymmetry allows for tree level $e \rightarrow \tau$ conversion mediated by squarks; this suggests that large cross sections perhaps may be expected. Furthermore, depending on the models which give rise to the effective operators discussed above, there may be large log enhancements in the charge radius contribution to photon exchange $e \rightarrow \tau$ which could overcome the limits on the four lepton operators.

Finally, we observe that many experiments have over many years placed limits on a wide variety of flavor-violating processes. Many of these experiments constrain the leptoquark parameter space, as analyzed in [1238. Updated limits from experimental searches for other flavor-violating processes may exist and still need to be considered in analyzing the potential of the EIC (and LHC) to search for LQ-mediated LFV events. Such limits may also be relevant for non-LQ scenarios. Improved limits from ongoing and future experiments searching for $\operatorname{LFV}(1,2)$ processes also need to be included, depending on the context for the $e \rightarrow \tau$ analysis.

This concludes the discussion of the theoretical analysis of leptoquark-induced $e \rightarrow \tau$ conversion in deep-inelastic scattering at the EIC. The analysis so far has been optimistic and disregarded important experimental considerations that would impact a search for $e \rightarrow \tau$ events. The next several sections address the questions of SM backgrounds and $\tau$ detection.

### 6.3.5 Experiment I: Standard Model Backgrounds \& the Analysis Strategy

In this section, we discuss the main SM processes that could mimic the $\operatorname{LFV}(1,3)$ signal at the EIC. In the SM, ep scattering is caused by the exchange of an electroweak gauge boson between the electron and a quark inside the proton. Photon exchange dominates when
the momentum transfer $Q$ is low, but the amplitude of weak gauge bosons becomes more important as $\left|Q^{2}\right|$ approaches $M_{W^{ \pm}}^{2}$ and $M_{Z^{0}}^{2}$. Standard Model NC and CC DIS processes are shown in figure 6.10. The EIC acceptance from the beampipe $\left(0.1^{\circ}<\theta<179.9^{\circ}\right)$ restricts all EIC kinematics to $Q^{2}>0.01 \mathrm{GeV}^{2}$ [1239]. This cut was implemented in the SM simulations at low momentum transfer. However, we focused our SM background analysis on events with very high $Q^{2}$ since a cut of $Q^{2}>1000 \mathrm{GeV}^{2}$ was used in all simulations involving leptoquarks (given the range of LQ masses chosen, see table 6.6).


Figure 6.10. NC and CC DIS diagrams.
Ignoring rare processes, the final state $\tau$ in the $\operatorname{LFV}(1,3)$ event can decay in three different ways: electronic channel, muonic channel, and hadronic channel. Like previous searches done at HERA [1223, 1224, we consider five different SM events whose final states could be misidentified with a decaying $\tau$ : NC DIS, CC DIS, photoproduction, lepton-pair production, and real W boson production.

SM processes lead to final state particles that could be misidentified as our candidate $\tau$. In other words, they produce particles that leave tracks in the detector that look like the leptons or hadrons produced in a $\tau$ decay. However, the geometry of the SM events and the $\operatorname{LFV}(1,3)$ events do differ. Indeed, the identified $\tau$ lepton in an $e p \rightarrow \tau X$ conversion must be back-to-back in azimuth with the hadronic sector $X$. In addition, the angular distribution in the $\theta$ direction of the decay products of scalar LQs, vector LQs, and SM DIS background will differ because their corresponding cross sections have a different $y$ dependence 5 By inspecting equations (6.23) and (6.24) we can see that in the s-channel (see figure 6.5) vector LQs are distributed according to $d \sigma / d y \propto(1-y)^{2}$, whereas scalar LQs decay isotropically (flat $d \sigma / d y$ distribution) in their rest frame (and vice-versa in the u-channel). In contrast, NC DIS events have $d \sigma / d y \propto y^{-1 / 2}$, and this difference between LQ and SM $y$ spectra could be exploited to identify background DIS events 1240 .

At the detector level, the events in all channels at the EIC must be accepted by a trigger for a large imbalance in the transverse energy flow. The energy flow summation runs over all energy deposits in the calorimeters and missing transverse momentum is associated to the neutrinos that escape the detector without any energy deposit. In this initial analysis, the missing transverse momentum $p_{T}^{\text {miss }}$ is defined as:

$$
\begin{equation*}
p_{T}^{m i s s}=\sqrt{\left(\sum P_{x, i}\right)^{2}+\left(\sum P_{y, i}\right)^{2}} \tag{6.31}
\end{equation*}
$$

where $i$ runs over all final state particles in an event, excluding all neutrinos.
PYTHIA 6.4.23 is used to generate all SM events with the CTEQ 5L parametrization

[^286]of the parton distribution functions of the proton 1241 . Initial and final state radiation are included. No GEANT simulation of the EIC detector has been used. Two different energies are chosen for the ep MC simulations: $20 \times 325 \mathrm{GeV}$ with $\sqrt{s}=161.25 \mathrm{GeV}$ and $10 \times 250 \mathrm{GeV}$ with $\sqrt{s}=100.01 \mathrm{GeV}$. Although not directly relevant for the conclusions of this topological study, we allowed ourselves the possibility of gathering a total integrated luminosity of $1000 \mathrm{fb}^{-1}$ as suggested on this workshop's web page [1239].

## Standard Model Event Generation

NC DIS: $(e p \rightarrow e X)$
NC DIS events are mediated by a photon or a $Z^{0}$ boson, and the final state includes an electron. The final state event topology of the tau electronic decay $\left(\tau \rightarrow e \nu_{e} \nu_{\tau}\right)$ is therefore very similar to that of high $Q^{2}$ NC DIS. By energy-momentum conservation the $\sum\left(E-P_{z}\right)$ distribution for NC DIS events is peaked at $2 E_{0}$, where $E_{0}$ is the electron beam energy (10 or 20 GeV ). We can also select NC events by implementing an upper and lower cut to the quantity $\sum\left(E-P_{z}\right)$ measured. In contrast, the $\tau$ decay exhibits a large missing transverse momentum due to the neutrinos in the decay.

CC DIS: $(e p \rightarrow \nu X)$
CC DIS events are mediated by a $W^{ \pm}$boson and are characterized by high missing transverse momentum $p_{T}^{m i s s}$ and higher $Q^{2}$.

Photoproduction: $(\gamma p \rightarrow X)$
Events from photoproduction processes occur in the low $Q^{2}$ limit and may contribute to the final selection if a narrow hadronic jet fakes the tau signature or is misidentified as an electron. For $\gamma p$ events simulated with PYTHIA, the photon can be either direct (point-like) or resolved (VMD and GVMD/anomalous). A photon is assumed to be direct (point-like) when it can only interact in processes which explicitly contain the incoming photon [81], such as $f_{i} \gamma \rightarrow f_{i} g$. A photon is considered to be resolved when it interacts through its constituent quarks and gluons. Each photoproduction subprocess leads to a different event structure and has a cross section that depends strongly on the virtuality of the photon. For high virtualities (high $Q^{2}$ ), DIS events dominate, and the photon is very virtual $\left(\gamma^{*}\right)$. For very low $Q^{2}$, however, the photon can be treated as real and can have a partonic structure that can interact in different ways with the proton's quark (e.g., resolved photoproduction).

However, the LFV processes were simulated with a $Q^{2}>1000 \mathrm{GeV}^{2}$ cut and hence the SM photoproduction background will automatically be reduced to zero. As table 6.4 below suggests, most of the background that concerns us is therefore in the DIS region where the photon is very virtual.

## Lepton-pair Production: $\left(e p \rightarrow e l^{+} l^{-} X\right)$

Lepton-pair production events contribute to the background because they may lead to high momentum leptons in the final state. An analysis of the event geometry is required to avoid misidentifying the three pencil-like tracks in the tau decay with the tracks left

| Subprocess | \% of tot. events, $Q^{2}>0.01$ | \% of tot. events, $Q^{2}>1000$ |
| :---: | :---: | :---: |
| VMD | 61.56 | 0 |
| Direct | 11.28 | 0 |
| Anomalous | 9.05 | 0 |
| DIS $\left(\gamma^{*} q \rightarrow q\right)$ | 18.11 | 100 |

Table 6.4. Event statistics for photoproduction/DIS subprocesses simulated at $20 \times 325 \mathrm{GeV}$ with $Q^{2}>0.01 \mathrm{GeV}^{2}$ and $Q^{2}>1000 \mathrm{GeV}^{2}$.
by $l^{+}, l^{-}$and $X$ when the scattered electron is missed. The background samples include $e^{+} e^{-}, \tau^{+} \tau^{-}$and $\mu^{+} \mu^{-}$production. The simulation of these processes was not included in this analysis due to its very low cross section given the chosen EIC energy range. However, they can be included in the future using a better suited generator with improved efficiency compared to PYTHIA.

## W Production: $(e p \rightarrow e W X)$

Real W boson production leads to final states with isolated leptons with high transverse momentum. The simulated W production samples include hadronic W decays (which can fake a tau decay) and leptonic ( $\left.l \bar{\nu}_{l}\right)$ decays that contribute to the missing transverse momentum and could potentially produce a non-LFV $\tau$. However, the cross section of this process $\left(2.449 \times 10^{-13} \mathrm{mb}\right.$ for $10 \times 250$ and $5.343 \times 10^{-11} \mathrm{mb}$ for $\left.20 \times 325\right)$ at EIC energies and luminosities is negligible.

## Results

Figures 6.11 and 6.12 include all SM processes. Shown are the $p_{T}^{m i s s}$ and acoplanarity $\Delta \phi_{\text {miss- }}$ jet found in events due to missing neutrinos. The plots are made for two different beam energy combinations (top and bottom). It is apparent that beam energies do not matter, the plots are very similar. Two different $Q^{2}$ conditions were studied: left and right, which isolate predominantly high and low $Q^{2}$ events, respectively. With no $Q^{2}$ cut, the event sample is dominated by low $Q^{2}$ photo-production background. If a cut of $Q^{2}>1000 \mathrm{GeV}^{2}$ is made the EW-physics (W) events become apparent. Figure 6.12 shows the acoplanarity $\Delta \phi_{\text {miss- }}$ jet , the angle between the reconstructed $\tau$-jet direction and the missing momentum direction (presumably the neutrinos in the primary collision) for the two different energies and virtualities. The figures also reveal that the shapes of the curves are very similar for the two different center-of-mass energies.

The particles in table 6.3.5 are primarily produced from the decays of hadrons in the hadronic sector $X$; e.g., $\tau \mathrm{s}$ can be produced from $D_{s}$ meson decay, but also include leptons from the processes mentioned above. The low $P_{T}$ suggests that these background particles can be partially avoided by restricting the kinematics phase space to high $Q^{2}$ and high transverse momentum.


Figure 6.11. $p_{T}^{m i s s}$ at $10 \times 250$ and $20 \times 325 \mathrm{GeV}$ with low $Q^{2}$ and $Q^{2}>1000 \mathrm{GeV}^{2}$.


Figure 6.12. Acoplanarity $\Delta \phi_{\text {miss }-\tau \text { jet }}$ at $10 \times 250$ and $20 \times 325 \mathrm{GeV}$ with low $Q^{2}$ and $Q^{2}>1000$ $\mathrm{GeV}^{2}$.

### 6.3.6 Experiment II: Leptoquark Simulation Study

## Type of Leptoquark Studied: Parameter Space

In this work we present the distribution of $p_{T}^{\text {miss }}$ generated from a LFV signal Monte Carlo sample of the leptoquark $\tilde{S}_{1 / 2}^{L} \frac{6}{6}$ The mass of the leptoquark is determined from the ratios $z \equiv \frac{\lambda_{i} \lambda_{j}}{M^{2}}$. The smallest value of the these ratios 1242 which the EIC will potentially probe are listed in table6.6. The LFV signal Monte Carlo events were generated using a LQ generator called "LQGENEP" [1243]. LQGENEP is a LQ generator for electron/positronproton scattering which simulates processes involving LQ production and exchange using the BRW [1225] effective model. The generator is interfaced with the PYTHIA event generator. The value of $\lambda_{i}=\lambda_{j}=0.3$ is taken throughout this study. The values of $\lambda$ are correlated with $z$ through their relation to the mass of the leptoquarks, $M_{L Q}$.

[^287]| Particle ID | $N_{1}$ | $N_{2}$ | $\mathbf{1 0 \times 2 5 0}$ | $\mathbf{2 0 \times 3 2 5}$ |
| :---: | :---: | :---: | :---: | :---: |
| $\tau^{-}$ | 531 | 316 | $p_{T}<4, \theta_{p} \sim 2$ | $p_{T}<4, \theta_{p} \sim 2$ |
| $\tau^{+}$ | 512 | 385 | $p_{T}<4, \theta_{p} \sim 1$ | $p_{T}<4, \theta_{p} \sim 1$ |
| $\mu^{-}$ | 38771 | 27849 | $p_{T}<2, \theta_{p} \sim 4$ | $p_{T}<2, \theta_{p} \sim 4$ |
| $\mu^{+}$ | 38691 | 27523 | $p_{T}<2, \theta_{p} \sim 4$ | $p_{T}<2, \theta_{p} \sim 4$ |
| $\nu_{\tau}$ | 1043 | 701 | $p_{T}<1, \theta_{p} \sim 4$ | $p_{T}<1, \theta_{p} \sim 4$ |
| $\nu_{\mu}$ | 37200 | 26170 | $p_{T}<2, \theta_{p} \sim 4$ | $p_{T}<2, \theta_{p} \sim 4$ |
| $\nu_{e}$ | 38343 | 27255 | $p_{T}<2, \theta_{p} \sim 4$ | $p_{T}<2, \theta_{p} \sim 4$ |
| $\overline{\nu_{\tau}}$ | 1043 | 701 | $p_{T}<1, \theta_{p} \sim 4$ | $p_{T}<1.5, \theta_{p} \sim 4$ |
| $\overline{\nu_{\mu}}$ | 37280 | 26496 | $p_{T}<2, \theta_{p} \sim 4$ | $p_{T}<2, \theta_{p} \sim 4$ |
| $\overline{\nu_{e}}$ | 38836 | 28004 | $p_{T}<2, \theta_{p} \sim 3$ | $p_{T}<2, \theta_{p} \sim 4$ |

Table 6.5. Statistics of selected SM background particles for 10 million $e^{-} p$ collisions generated with PYTHIA. $N_{1}$ and $N_{2}$ are the number of times the particle is produced out of the 10 million events at energies of $20 \times 325 \mathrm{GeV}$ and $10 \times 250 \mathrm{GeV}$ respectively. $\theta_{p}$ is the peak of the particle's polar angle distribution in degrees with a FWHM $\sim 11^{\circ}$ and $p_{T}$ is the transverse momentum in GeV . All $\phi$ distributions are flat.

| $\left(q_{i} q_{j}\right)$ | $z\left(\mathrm{TeV}^{-2}\right)$ | Mass $(\mathrm{GeV})$ |
| :---: | :---: | :---: |
| 11 | 0.024 | 1936.5 |
| 13 | 0.03 | 1732.0 |
| 22 | 0.039 | 1519.1 |
| 23 | 0.047 | 1383.8 |
| 31 | 0.03 | 1732.0 |
| 32 | 0.06 | 1224.7 |
| 33 | 0.084 | 1035.1 |

Table 6.6. The initial and final quark flavors $\left(q_{i} q_{j}\right)$ in the subprocess $e q_{i} \rightarrow \tau q_{j}$, the ratio $z$ and the mass of the LQ for $\lambda_{i}=\lambda_{j}=0.3$.

## Leptoquark Event Characterization

Electron-to-tau events were generated using the LFV generator LQGENEP for two EIC energies, namely, $10 \times 250 \mathrm{GeV}$ and $20 \times 325 \mathrm{GeV}$, in ep scattering. These events were restricted to sub-processes with a specific intermediary BRW LQ, $\tilde{S}_{1 / 2}^{L}$. The kinematic region was restricted to $Q^{2}>1000 \mathrm{GeV}^{2}$ and $y>0.1$.

## Electronic \& muonic $\tau$ decays

The leptonic decays of the tau, $\tau \rightarrow e \bar{\nu}_{e} \nu_{\tau}, \mu \bar{\nu}_{\mu} \nu_{\tau}$, were studied. Background for these events is present from SM neutral current events in ep DIS. The $p_{T}^{m i s s}$ distribution for $10 \times 250$ and $20 \times 325$ are shown in figure 6.3 .6 (left) and (right), respectively. The plots shown are for electron final states. The muon final state plots are identical. The different panels indicate the $p_{T}^{\text {miss }}$ spectrum for each combination of quarks $i, j$ involved. The $p_{T}^{\text {miss }}$ spectrum is wider at higher center-of-mass energies, but otherwise the spectra are generally similar.


Figure 6.13. Missing transverse momentum in the electronic $\tau$ decay channel in the ep scattering with 10 x 250 (left) and $20 \times 325$ (right) energies and the ratios, $z$, from table 6.6 for $\left(q_{i} q_{j}\right) \equiv 13,22,23,31,32$ and 33. The lepton-quark couplings are $\lambda_{i}=\lambda_{j}=0.3$.

## Hadronic $\tau$ decays

The hadronic decay of high- $P_{T} \tau$ leptons results in a characteristic narrow "pencillike" jet with three pions. The event $e p \rightarrow \tau X$ would look like a a di-jet event with one narrow and one wide/high multiplicity jet. The jet associated with the $\tau$ decay is narrow. Thus one narrow and one wide jet in a di-jet event is a potential candidate for the signal. Various standard algorithms are used to identify such events [1224]. We did not simulate the detector response - this is a topic for a future detector study - but we studied the event characteristics and topology for such events.

The $p_{T}^{\text {miss }}$ distribution for 10x250 and 20x325 are shown in figure 6.3.6 (left) and (right), respectively. Also plotted is the acoplanarity, $\Delta \phi_{\text {miss }-\tau j e t}$, between the $\tau$-jet and the missing transverse momentum. $\Delta \phi_{\text {miss- }- \text { jet }}$ for the EIC energies $10 x 250$ and 20 x 325 , shown in figure 6.3 .6 (left) and (right) respectively. Figure 6.3 .6 shows the same results as previous two figures but with an additional requirement of $\Delta \phi_{\text {miss- } j \text { jet }}$ below $20^{\circ}$. A small $\Delta \phi_{\text {miss- }}$ jet requirement means that the missing transverse momentum in the event, in the form of a $\tau$ neutrino, is aligned with the $\tau$ jet. These should be the events in which the $\tau$ decayed with neutrinos in the final state.

### 6.3.7 Experiment III: Concluding Remarks

We have studied the topological differences between events in the SM and a BRWleptoquark extension of the SM. Leptoquark searches in electron-hadron machines are sensitive to the ratio of the product of coupling constant to the square of the leptoquark mass. Motivated by recent theoretical expectations first presented in [1226] and summarized above in section 6.3.2, we have studied this for a range of leptoquark masses. While we studied the topologies of leptoquark-mediated transitions between the electron and all three generations of charged leptons, we limit our comments to the $\operatorname{LFV}(1,3)$ transition, for now.


Figure 6.14. Missing transverse momentum in the hadronic $\tau$ decay channel in the ep scattering with $10 \times 250$ (left) and $20 \times 325$ (right) energies and the ratios, $z$, from table 6.6 for $\left(q_{i} q_{j}\right) \equiv 13,22,23,31,32$ and 33. The lepton-quark couplings are $\lambda_{i}=\lambda_{j}=0.3$.


Figure 6.15. The acoplanarity, $\Delta \phi_{\text {miss- }}$ jet , between the $\tau-j e t$ and the missing transverse momentum in the hadronic $\tau$ decay channel in the ep scattering with $10 \times 250$ (left) and 20 x 325 (right) energies respectively and the ratios, $z$, from table 6.6 for $\left(q_{i} q_{j}\right) \equiv 13,22,23,31,32$ and 33.The leptonquark couplings are $\lambda_{i}=\lambda_{j}=0.3$.


Figure 6.16. The acoplanarity, $\Delta \phi_{\text {miss- }-j e t}$, between the $\tau-j e t$ and the missing transverse momentum in the hadronic $\tau$ decay channel in the ep scattering with $10 \times 250$ (left) and $20 \times 325$ (right) energies respectively and the ratios, $z$, from table 6.6 for $\left(q_{i} q_{j}\right) \equiv 13,22,23,31,32$ and 33 . The lepton-quark couplings are $\lambda_{i}=\lambda_{j}=0.3 . \Delta \phi_{m i s s-\tau j e t}$ is required to be below $20^{\circ}$.

## Observations

The topological features of a SM event that produces a $\tau$ lepton which decays and an event in which a $\tau$ is created as a decay of a leptoquark are distinct in two different variables routinely studied in colliders. They are: 1) $p_{T}^{\text {miss }}$ spectrum, transverse missing momentum in such an event, and 2) $\Delta \phi_{\text {miss- }}$ jet , defined as the transverse angle $\phi$ between the $\tau$ created in the event and the vector direction of missing momentum.

As shown in figure 6.17, the $p_{T}^{\text {miss }}$ spectrum is extremely narrow for SM events with final state leptonic or hadronic decays of the $\tau$ created in the collisions. This implies that the neutrinos released in the decay of the SM-produced $\tau$ are boosted in the direction of the $\tau$ and hardly any noticeable transverse momentum is lost. In contrast, the $\tau$ produced in a leptoquark decay tends to have a larger spread in the $p_{T}^{\text {miss }}$ spectrum. These general features of the $p_{T}^{m i s s}$ spectra do not depend on the center-of-mass of the collision: the top histograms in figure 6.17 correspond to 100 GeV center-of-mass energy, while on the bottom they correspond to 160 GeV . Note that these plots are not normalized amongst themselves.

Figure 6.18 shows the acoplanarity plots, the angle between the $\tau$-jet in the event and the missing momentum vector reconstructed in the transverse plane using all other observable hadronic and leptonic activity (whether part of a jet or not). The left plots at each center-of-mass energy are unnormalized acoplanarity distributions showing that the SM events are distributed widely over the $\phi$ range, while the leptoquark-produced $\tau$ jets are narrowly peaked at $180^{\circ}$. If a proximity requirement cut of $20^{\circ}$ is made - meaning that the missing neutrinos were very close in $\phi$ angle with the direction of the generated $\tau$ - the distribution switches sides, indicating two categories of such events (the plots on the right of figure). Again, the top two histograms are for 100 GeV center-of-mass energy and the bottom are for 160 GeV . They show no differences based on these center-of-mass energies. This feature by itself will be less deterministic of the event topology of the leptoquarks, but we expect (as was done in previous searches [1223]) the $p_{T}^{\text {miss }}$ spectrum and the acoplanarity distributions together will be utilized in a maximum likelihood or neural network analysis to search for excesses seen in future EIC events.


Figure 6.17. SM and LQ (both hadronic and electronic channels) $p_{T}^{m i s s}$ at $10 \times 250$ and $20 \times 325 \mathrm{GeV}$ with $Q^{2}>1000 \mathrm{GeV}^{2}$. These plots are not normalized amongst themselves.


Figure 6.18. Acoplanarity $\Delta \phi_{\text {miss }, \tau \text { jet }}$ at $10 \times 250$ and $20 \times 325 \mathrm{GeV}$ with $Q^{2}>1000 \mathrm{GeV}^{2}$. The two plots in the right side have a $\Delta \phi<20^{\circ}$ cut implemented on the LQ simulation. In this case, the LQ preserves the quark flavor: $\left(q_{i}=1 q_{j}=1\right)$. These plots are not normalized amongst themselves.

## Outlook

The study we performed is only a beginning. The estimates made in the theoretical motivation in section 6.3.2 and [1226 assume a $100 \%$ efficiency of final state leptonic and hadronic decay reconstruction of the $\tau$ created in the final state. The experimental publications [1223, 1224 indicate that their detailed simulation of the H 1 detector resulted in a range of $7 \%$ to $15 \%$ in the reconstruction efficiency of the $\tau$ in those final states. BELLE and BaBar detectors have reported higher efficiencies reaching about $20 \%$. It is reasonable to assume that a future EIC detector may be able to achieve at least that. Assuming this we note that the luminosity requirements stated in section 6.3.2 and [1226] for the EIC to probe $e \rightarrow \tau$ cross sections at the level stated are an underestimate by about 10-to- 5 times. This means at 90 GeV center-of-mass, the stated $10 \mathrm{fb}^{-1}$ could be as high as 100 or as low as $50 \mathrm{fb}^{-1}$.

The studies we performed were based on HERA studies in which the collision energies were about 300 GeV in the center-of-mass frame. The efficiencies of some cuts and selection criteria would certainly be better at those energies than at the EIC 100 and 160 GeV center-of-mass energies, so the cut efficiencies may not transfer exactly as it has been assumed in these estimates. However, it is not unreasonable to assume that a similar but equally (if not more) efficient set of cuts and analysis techniques may be eventually found for this search at the future EIC.

The group now formed hopes to continue these studies with detailed detector simulation as it will become available in near future.

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## Chapter 7

## Experimental aspects

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# 7.1 High-energy high-luminosity electron-ion collider eRHIC 

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### 7.1.1 Introduction

In this paper, we describe a future electron-ion collider (EIC), based on the existing Relativistic Heavy Ion Collider (RHIC) hadron facility, with two intersecting superconducting rings, each 3.8 km in circumference [1244]. The replacement cost of the RHIC facility is about two billion US dollars, and the eRHIC will fully take advantage and utilize this investment. We plan adding a polarized $5-30 \mathrm{GeV}$ electron beam to collide with variety of species in the existing RHIC accelerator complex, from polarized protons with a top energy of 325 GeV , to heavy fully-stripped ions with energies up to $130 \mathrm{GeV} / u$.

Brookhavens innovative design, (figure 1), is based on one of RHICs hadron rings and a multi-pass energy-recovery linac (ERL). Using the ERL as the electron accelerator assures high luminosity in the $10^{33}-10^{34} \mathrm{~cm}^{-2} \sec ^{-1}$ range, and for the natural staging of eRHIC, with the ERL located inside the RHIC tunnel. eRHIC will provide electron-hadron collisions in up to three interaction regions. We detail eRHICs performance in subsection 7.1.2,

Since the first paper on eRHIC in 2000, its design has undergone several iterations. Initially, the main eRHIC option (the so-called ring-ring, RR, design) was based on an electron ring, with the linac-ring (LR) option as a backup. In 2004, we published the detailed "eRHIC 0th-Order Design Report" including a cost-estimate for the RR design [1245]. After detailed studies, we found that an LR eRHIC has about a 10 -fold higher luminosity than the RR. Since 2007, the LR, with its natural staging strategy and full transparency for polarized electrons, became the main choice for eRHIC. In 2009, we completed technical studies of the design and dynamics for MeRHIC with 3-pass 4-GeV ERL. We learned much from this evaluation, completed a bottom-up cost estimate for this $\$ 350 \mathrm{M}$ machine, but then shelved the design.

In the same year, we turned again to considering the cost-effective, all-in-tunnel sixpass ERL for our design of the high-luminosity eRHIC (figure 7.1). In it, electrons from the polarized pre-injector will be accelerated to their top energy by passing six times through two SRF linacs. After colliding with the hadron beam in up to three detectors, the e-beam will be decelerated by the same linacs and dumped. The six-pass magnetic system with small-gap magnets [1246] will be installed from the start. We will stage the electron energy from 5 GeV to 30 GeV stepwise by increasing the lengths of the SRF linacs.

We considered several IR designs for eRHIC. The latest one, with a 10 mrad crossing angle and $\beta^{*}=5 \mathrm{~cm}$, takes advantage of newly commissioned $N b_{3} S n$ quadrupoles [1247]. Subsection 7.1.3 details the eRHIC lattice and the IR layout.

The current eRHIC design focuses on electron-hadron collisions. If justified by the EIC physics, we will add a 30 GeV polarized positron ring with full energy-injection from the


Figure 7.1. (a) Layout of the ERL-based, all-in-RHIC-tunnel, $30 \mathrm{GeV} \times 325 \mathrm{GeV}$ high-energy high-luminosity eRHIC. (b) Location of eRHICs six recirculation arcs in the RHIC tunnel.
eRHIC ERL. This addition to the eRHIC facility provides for positron-hadron collisions, but at a significantly lower luminosity than those attainable in the electron-hadron mode.

As a novel high-luminosity EIC, eRHIC faces many technical challenges, such as generating 50 mA of polarized electron current. eRHIC also will employ coherent electron cooling (CeC) 1248 for the hadron beams. Staff at BNL, JLab, and MIT are pursuing vigorously an R\&D program for resolving addressing these obstacles. In collaboration with Jlab, BNL plans experimentally to demonstrate CeC at the RHIC. We discuss the structure and the status of the eRHIC R\&D in subsection 7.1.4.

### 7.1.2 Main eRHIC parameters

eRHIC is designed to collide electron beams with energies from 5 - to $30-\mathrm{GeV} 1$ with hadrons, viz., either with heavy ions with energies from $50-$ to $130-\mathrm{GeV}$ per nucleon, or with polarized protons with energies between $100-$ and $325-\mathrm{GeV}$. Accordingly, eRHIC will cover the C.M. energy range from $44.7-$ to $197.5-\mathrm{GeV}$ for polarized e-p, and from 31.6- to $125-\mathrm{GeV}$ for electron heavy-ion-collisions.

Several physics and practical considerations influenced our choice of beam parameters for eRHIC. Some of these limitations, such as the intensity of the hadron beam, the space charge and beam-beam tune shift limits for hadrons, come from experimental observations at RHIC or other hadron colliders. Some of them, for example $\beta^{*}=5 \mathrm{~cm}$ for hadrons, are at the limits of current accelerator technology, while others are derived either from practical or cost considerations. For example, from considering the operational costs, we limit the electron beam's power loss for synchrotron radiation to about 7 MW , corresponding to a 50 mA beam current at 20 GeV . Above 20 GeV , the electron beam's current will decrease in inverse proportion to the fourth power of energy, and will be restricted to about 10 mA at an energy of 30 GeV . It means that the luminosity of eRHIC operating with 30 GeV electrons will be a $1 / 5$ th of that with 20 GeV .

[^288]Since the ERL provides fresh electron bunches at every collision, the electron beam can be strongly abused, i.e., it can be heavily distorted during a collision. The only known effect that might cause a serious problem is the so-called kink instability. The ways of suppressing it within range of parameters accessible by eRHIC is well-understood [1249] and it no longer presents a problem.

We list below some of our assumed limits and parameters:

1. Bunch-intensity limits:
a. For protons: $210^{11}$
b. For Au ions: $1.210^{9}$
2. Electron-current limits:
a. Polarized current: 50 mA
b. Un-polarized current: 250 mA
3. Minimum $\beta^{*}=5 \mathrm{~cm}$ for all species
4. Space-charge tune shift for hadrons: $\leq 0.035$
5. Proton (ion) beam-beam parameter: $\leq 0.015$
6. Bunch length (with coherent electron-cooling):
a. Protons: 8.3 cm at energies below $250 \mathrm{GeV}, 4.9 \mathrm{~cm}$ at 325 GeV
b. Au ions: 8.3 cm in all energy ranges
7. Synchrotron radiation intensity limit is defined as that of a 50 mA beam at 20 GeV
8. Collision rep-rate $\leq 50 \mathrm{MHz}$.

The limitations on luminosity resulting from various considerations are involved. The main trend is that eRHIC's luminosity does not depend on the electron beam's energy (below 20 GeV ) and reaches its maximum at the hadron beam's highest energy. We mentioned the exception for energies of electrons above 20 GeV . The top eRHIC performance for various species is shown in table 7.1,

Table 7.2 lists the luminosity of a polarized electron-proton collision for a set of electronand proton-energies. Table 7.3 contains this information for a polarized electron beam colliding with Au ions, while tables 7.4 and 7.5 provide data for the case of unpolarized electrons.

An additional major parameter describing eRHIC's overall performance is its expected average luminosity. Since the plans for eRHIC are to use coherent electron cooling to control the parameters of hadron beam, its lifetime will be affected only by scattering on residual gas, and by burn-off in collisions with electrons. Hence, the hadron beam's luminosity lifetime could be as long as a few days, and, in the most likely scenario, the average delivered luminosity will be determine by the reliability of RHIC systems. Hence we anticipate that the average luminosity will be $\sim 70 \%$ of that listed in the tables.

### 7.1.3 The eRHIC interaction region

The current high-luminosity eRHIC IR design incorporates a 10 mrad crab-crossing scheme; thus, hadrons traverse the detector at a 10 mrad horizontal angle, while electrons go straight through. Figure 7.2 plots this scheme. The hadron beam is focused to $\beta^{*}=5 \mathrm{~cm}$ by a special triplet wherein the first magnet is a combined function magnet ( 1.6 m long with 2.23 T magnetic fields and a - $109 \mathrm{~T} / \mathrm{m}$ gradient). It has two functions; it focuses the hadron beam while bending it 4 mrad . Two other quadrupoles do not bend the hadron beam but serve only for focusing. Importantly, all three magnets provide zero magnetic fields along the electron beam's trajectory. Quadrupoles for this IR require very high gradients, and can be built only with modern superconducting technology [1247, 1250]

|  | e | p | ${ }^{2} \mathrm{He}^{3}$ | ${ }^{79} \mathrm{Au}^{197}$ | ${ }^{92} \mathrm{U}^{238}$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| Energy, GeV | $5-20$ | 325 | 215 | 130 | 130 |
| CM energy, GeV |  | $80-161$ | 131 | 102 | 102 |
| Number of bunches or distance be- <br> tween bunches | 74 nsec | 166 | 166 | 166 | 166 |
| Bunch intensity (nucleons), $10^{11}$ | 0.24 | 2 | 3 | 3 | 3.15 |
| Bunch charge, nC | 3.8 | 32 | 30 | 19 | 20 |
| Beam current, mA | 50 | 420 | 390 | 250 | 260 |
| Normalized emittance of hadrons <br> $95 \%$, mm $\cdot$ mrad |  | 1.2 | 1.2 | 1.2 | 1.2 |
| Normalized emittance of elec- <br> trons, rms, mm $\cdot$ mrad |  | $5.8-23$ | $7-35$ | $12-57$ | $12-57$ |
| Polarization, \% | 80 | 70 | 70 | none | none |
| RMS bunch length, cm | 0.2 | 4.9 | 8.3 | 8.3 | 8.3 |
| $\beta^{*}$, cm | 5 | 5 | 5 | 5 | 5 |
| Luminosity per nucleon, $10^{34}$ <br> $\mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ |  | 1.46 | 1.39 | 0.86 | 0.92 |

Table 7.1. Projected eRHIC luminosity for various hadron beams at top energy.

| Electrons Protons | 100 GeV | 130 GeV | 250 GeV | 325 GeV |
| :---: | :---: | :---: | :---: | :---: |
| 5 GeV | $0.62 \cdot 10^{33}$ | $1.4 \cdot 10^{33}$ | $9.7 \cdot 10^{33}$ | $15 \cdot 10^{33}$ |
| 10 GeV | $0.62 \cdot 10^{33}$ | $1.4 \cdot 10^{33}$ | $9.7 \cdot 10^{33}$ | $15 \cdot 10^{33}$ |
| 20 GeV | $0.62 \cdot 10^{33}$ | $1.4 \cdot 10^{33}$ | $9.7 \cdot 10^{33}$ | $1.5 \cdot 10^{33}$ |
| 30 GeV | $0.12 \cdot 10^{33}$ | $0.3 \cdot 10^{33}$ | $1.9 \cdot 10^{33}$ | $3 \cdot 10^{33}$ |

Table 7.2. Projected eRHIC luminosity (in $\mathrm{cm}^{-2} \mathrm{sec}^{-1}$ ) for polarized electron-proton collisions.

| Electrons Au ions | $50 \mathrm{GeV} / \mathrm{u}$ | $75 \mathrm{GeV} / \mathrm{u}$ | $100 \mathrm{GeV} / \mathrm{u}$ | $130 \mathrm{GeV} / \mathrm{u}$ |
| :---: | :---: | :---: | :---: | :---: |
| 5 GeV | $0.49 \cdot 10^{33}$ | $1.7 \cdot 10^{33}$ | $3.9 \cdot 10^{33}$ | $8.6 \cdot 10^{33}$ |
| 10 GeV | $0.49 \cdot 10^{33}$ | $1.7 \cdot 10^{33}$ | $3.9 \cdot 10^{33}$ | $8.610^{33}$ |
| 20 GeV | $0.49 \cdot 10^{33}$ | $1.710^{33}$ | $3.9 \cdot 10^{33}$ | $8.6 \cdot 10^{33}$ |
| 30 GeV | $0.1 \cdot 10^{33}$ | $0.34 \cdot 10^{33}$ | $0.8 \cdot 10^{33}$ | $1.7 \cdot 10^{33}$ |

Table 7.3. Projected eRHIC luminosity (in $\mathrm{cm}^{-2} \mathrm{sec}^{-1}$ ) for polarized electrons and $A u$ ions.

| Electrons Protons | 100 GeV | 130 GeV | 250 GeV | 325 GeV |
| :---: | :---: | :---: | :---: | :---: |
| 5 GeV | $3.1 \cdot 10^{33}$ | $5 \cdot 10^{33}$ | $9.7 \cdot 10^{33}$ | $15 \cdot 10^{33}$ |
| 10 GeV | $3.1 \cdot 10^{33}$ | $5 \cdot 10^{33}$ | $9.7 \cdot 10^{33}$ | $15 \cdot 10^{33}$ |
| 20 GeV | $0.62 \cdot 10^{33}$ | $1.4 \cdot 10^{33}$ | $9.7 \cdot 10^{33}$ | $15 \cdot 10^{33}$ |
| 30 GeV | $0.12 \cdot 10^{33}$ | $0.3 \cdot 10^{33}$ | $1.9 \cdot 10^{33}$ | $3 \cdot 10^{33}$ |

Table 7.4. Projected eRHIC luminosity (in $\mathrm{cm}^{-2} \mathrm{sec}^{-1}$ ) for polarized protons and unpolarized electrons.

| Electrons Au ions | $50 \mathrm{GeV} / \mathrm{u}$ | $75 \mathrm{GeV} / \mathrm{u}$ | $100 \mathrm{GeV} / \mathrm{u}$ | $130 \mathrm{GeV} / \mathrm{u}$ |
| :---: | :---: | :---: | :---: | :---: |
| 5 GeV | $2.5 \cdot 10^{33}$ | $8.3 \cdot 10^{33}$ | $11.4 \cdot 10^{33}$ | $18 \cdot 10^{33}$ |
| 10 GeV | $2.5 \cdot 10^{33}$ | $8.3 \cdot 10^{33}$ | $11.4 \cdot 10^{33}$ | $18 \cdot 10^{33}$ |
| 20 GeV | $0.49 \cdot 10^{33}$ | $1.710^{33}$ | $3.9 \cdot 10^{33}$ | $8.6 \cdot 10^{33}$ |
| 30 GeV | $0.1 \cdot 10^{33}$ | $0.34 \cdot 10^{33}$ | $0.8 \cdot 10^{33}$ | $1.7 \cdot 10^{33}$ |

Table 7.5. Projected eRHIC luminosity (in $\mathrm{cm}^{-2} \mathrm{sec}^{-1}$ ) for unpolarized electrons and Au ions.


Figure 7.2. Layout of the right side of eRHIC IR from the IP to the RHIC arc. The spin rotator is the first element of existing RHIC lattice remaining in place in this IR design.

This configuration guaranties the absence of harmful high-energy X-rays from synchrotron radiation. Furthermore, the electron beam is brought into the collision via a 130 meter long merging system (figure 7.3). The radiation from regular bending magnets would be absorbed. The last 60 meters of the merging system use only soft bends: downwards magnets have strength of 84 Gs ( for 30 GeV beam ) and the final part of the bend used only 24 Gs magnetic field. Only 1.9 W of soft radiation from the later magnets would propagate through the detector.

One important factor in the IR design with low $\beta^{*}=5 \mathrm{~cm}$ is that the chromatism of the hadron optics in the IR should be controlled, which is reflected in the maximum $\beta$-function of the final focusing quadrupoles. Figure 7.4a shows the designed $\beta$ - and dispersion-functions for the hadron beam. The values of the $\beta$-function are kept under 2 km , and the chromaticity held at the level typical for RHIC operations with $\beta^{*} \sim 1 \mathrm{~m}$. We are starting full-fledged tracking of hadron beams in RHIC, including characterizing beam-beam effects and all known nonlinearities of RHIC magnets: we do not anticipate any serious chromatic effects originating from our IR design.


Figure 7.3. (a) Vertical trajectory of 30 GeV electron beam merging over 130 meters into the IP. (b) Spectra of the radiation from various part of the merger. Only 1.9 W of soft X-ray radiation will propagate through the detector; the absorbers intercept the rest of it.

Furthermore, we introduced the bending field in the first quadrupole for the hadrons thereby to separate the hadrons from the neutrons. Physicists considering processes of interest for EIC science requested our installing this configuration. Since the electrons are used only once, the optics for them is much less constrained. Hence, it does not present any technical- or scientific-challenges, and so we omit its description here.

Finally, beam-beam effects play important roles in eRHIC's performance. While we will control these effects on the hadron beam, i.e., we will limit the total tune shift for hadrons to about 0.015 , the electron beam is used only once and it will be strongly disrupted during its single collision with the hadron beam. Consequently, the electrons are strongly focused by the hadron beam (pinch effects), and the e-beam emittance grows by about a factor of two (disruption) during the collision. These effects, illustrated in figure 7.5, do not represent a serious problem, but will be carefully studied and taken into account in designing the optics and the aperture .

More details on the lattice and IR design are given in reference 1251 .


Figure 7.4. (a) Hadron beam's optics at the eRHIC IR. The $5 \mathrm{~cm} \beta^{*}$ is matched into the RHIC's arc lattice that starts about 60 m from the IR. (b) Tracking of hadrons with an energy deviation of $\pm 0.1 \%$ through the first four magnets at the IR.


Figure 7.5. (a) The optimized e-beam envelope during collision with the hadron beam in eRHIC; (b) Distribution of electrons after colliding with the hadron beam in eRHIC.

### 7.1.4 eRHIC R\&D

The list of the needed accelerator R\&D on eRHIC is quite extensive, ranging from the 50 mA CW polarized source [1252, 1253, 1254] to Coherent Electron Cooling [1248]. It includes designing and testing multiple aspects of SRF ERL technology in BNL's R\&D ERL (1255.

Coherent Electron Cooling (figure 7.6) promises to cool both ion beams by an order of magnitude (both transversely and longitudinally) in under half an hour. Traditional stochastic or electron cooling techniques could not satisfy this demand. Being a novel unverified technique, CeC will be tested in a proof-of-principle experiment at RHIC in a collaboration between scientists from BNL, JLab, and TechX [1256.

Another important R\&D effort, supported by an LDRD grant, focuses on designing and prototyping small-gap magnets and vacuum chamber for cost-effective eRHIC arcs [1246]. In addition to their energy efficiency and inexpensiveness, small-gap magnets assure
a very high gradient as room-temperature quadrupole magnets. Figure 7.7 shows two such prototypes; they were carefully tested and their fields were mapped using high-precision magnetic measurements. While the quality of their dipole field is close to satisfying our requirements, the quadrupole prototype was not manufactured to our specifications. We will continue this study, making new prototypes using various manufacturers and techniques.


Figure 7.6. Possible layout of RHIC CeC system cooling for both the yellow and blue beams.


Figure 7.7. (a) A prototype of eRHIC quadrupole with 1 cm gap; (b) Assembled prototype of eRHIC dipole magnet with 5 mm gap.

Another part of our R\&D encompasses testing the RHIC in the various modes that will be required for eRHIC's operation.

### 7.1.5 Conclusions and Acknowledgements

We are making steady progress in designing the high-energy, high-luminosity electronion collider eRHIC and plan to continue our R\&D projects and studies of various effects and processes. So far, we have not encountered a problem in our proposal that we cannot resolve. Being an ERL-based collider, eRHIC offers a natural staging of the electron beam's energy from 5-6 to 30 GeV . During this year, we will complete our cost estimate of all eRHIC stages.

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### 7.2 A Polarized Medium-Energy Electron-Ion Collider at JLab

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The conceptual design of MEIC, a polarized ring-ring electron-ion collider based on CEBAF, has been continuously optimized for best supporting the nuclear science program. MEIC covers a medium CM energy region up to 65 GeV (for 6 T superconducting dipole magnets) and achieves a luminosity of above $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ for one high-luminosity and one full-acceptance detectors. The unique compact figure- 8 shaped collider rings, designed to accommodate 3 to 11 GeV electrons and up to 96 GeV protons or 48 (38) $\mathrm{GeV} / \mathrm{u}$ for light (heavy) ions ( 128 GeV protons or $64(51) \mathrm{GeV} / \mathrm{u}$ light (heavy) ions for 8 T superconducting magnet), provide a great advantage for delivering and preserving high polarization of ion beams (including polarized deuterons) for collisions at multiple interaction points. The design is upgradable to accommodate 20 GeV electrons and about 250 GeV proton energies at a late stage, with luminosities up to $10^{35} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. The present focus of the Jefferson Lab accelerator team is to develop a coherent machine design that integrates all of the design features that have been explored over recent years, based upon state-of-the-art performance criteria. Various collider components including ion linac and boosters, spin rotators, and interaction regions have been designed and integrated into a unified design. These advances will be discussed in detail.

### 7.2.1 Introduction

Over the last decade, Jefferson Lab has been developing a conceptual design of an electron-ion collider for future nuclear physics research. This facility, fully utilizing the 12 GeV upgraded CEBAF, will provide collisions between polarized electrons and polarized light ions or unpolarized light to heavy ions up to lead over a wide CM energy range at multiple interaction points (IPs). Requirements of the science programs drive the design efforts to focus on achieving ultra-high luminosity $\left(10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}\right.$ or above) per detector, and high polarization (over $80 \%$ ) for both electron and light ion beams.

Our primary design focus at the present time is a Medium-energy Electron-Ion Collider (MEIC), with a CM energy up to 65 GeV , which covers electron energy up to 11 GeV , proton energy up to 96 GeV and ion energy up to 48 GeV per nucleon. It is considered as an optimal compromise between science, technology and project cost. We also maintain a well-defined upgrade capability to higher energies, ELIC, which can reach up to 20 GeV electron energy, and 250 GeV proton energy or 100 GeV /u heavy ion energies (typically, for heavy ions the proton number is about $40 \%$ of the atomic mass number). In both instances, high luminosity and high polarization remain the main design drivers.

The present MEIC design features a traditional ring-ring collider with a high luminosity at a level of $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ per detector, over up to three IPs, by taking full advantage of an electron beam from the upgraded 12 GeV CEBAF recirculated SRF linac. As a design concept, the high luminosity of MEIC is attained by utilizing high bunch repetition rate, crab-crossing colliding electron and ion beams with short bunch length and small transverse
emittances, and strong final focusing at collision points. Our choice of this luminosity concept was motivated by the remarkable success of two electron-positron colliders at KEK and SLAC B-factories, which had reached luminosities over $2 \times 10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. In a way, Jefferson Lab is poised to replicate the same success in a collider involving hadron beams. The new concept requires the colliding ion beams of MEIC to be very different from all existing or previously operated hadron colliders in terms of bunch intensity (very small), bunch length (very short), transverse emittances (very small) and repetition frequency (very high), while, at the same time, it pushes the final focusing parameter $\beta^{*}$ to be much smaller than what has been achieved in hadron colliders. To support such a conceptual design, extensive R\&D programs have been established at Jefferson Lab, supplemented by several external collaborations.

As a design strategy, we are taking a conservative technical position by limiting many MEIC design parameters within or close to the present state-of-the-art in order to minimize technical uncertainty. This conservative technical design will form a baseline for future design optimization guided by the evolution of the science program, technology innovations and $R \& D$ advances.

### 7.2.2 Baseline Design

The MEIC main parameters are summarized in table 7.2 .2 for a design point of 60 GeV proton and 5 GeV electron. Figure 7.8 presents luminosities as a function of CM energy for both proton and ions. In deriving this set of design parameters, we have imposed certain limits on several key machine or beam parameters in order to reduce technical risk and the accelerator R\&D challenges and to improve robustness of the design. These limits, based on largely previous lepton and hadron collider experiences and state-of-art of accelerator technologies, are:

- Average current of the stored beams are up to 1 A for protons/ions and 3 A for electrons,
- Electron synchrotron radiation power density is less than $20 \mathrm{~kW} / \mathrm{m}$,
- Peak bending field of ion superconducting dipole is no larger than 6 T ,
- The maximum betatron value at the beam extension area near an IP is no larger than 2.5 km ,
- Frequency of accelerating RF cavity in the electron ring is less than 1 GHz .

Also, different nuclear programs usually require different detector acceptances and arrangement of interaction regions (IR). While such detector requirements are still in a formation stage, we have considered two different types of IR designs, one for a full-acceptance detector (with 0.5 to 179.5 degree solid angular acceptance before the ion final focusing magnets, and the apertures of the latter sufficient to allow particles with angles up to 0.5 degrees to go through the bore of the magnet for downstream detection), the other for a high-luminosity detector. The key difference of the IR designs is a space between the collision point and the location of the first final focusing quad, and values of these distances for the two detectors are 7 m and 4.5 m respectively for ion beams, while the space for electron beams can be as low as 3 m for both cases. The relatively short distance of 4.5 m enables a further reduction of the final focusing $\beta^{*}$ to 8 mm , thus resulting in a more than a factor two increase of luminosity for that detector configuration as shown in table 7.2.2.

| Quantity | Unit | $p^{-}$beam | $e$ beam |
| :--- | :---: | :---: | :---: |
| Beam energy | GeV | 60 | 5 |
| Collision frequency | MHz | 749 |  |
| Particles per bunch | $10^{10}$ | 0.416 | 2.5 |
| Beam current | A | 0.5 | 3 |
| Polarization | $\%$ | $>70$ | $\sim 80$ |
| Energy spread | $10^{-3}$ | 0.3 | 0.71 |
| RMS bunch length | mm | 10 | 7.5 |
| Horiz. emit. (norm.) | $\mu \mathrm{m}$ | 0.35 | 53.5 |
| Vertical emit. (norm.) | $\mu \mathrm{m}$ | 0.07 | 10.7 |
| Horizontal $\beta^{*}$ | cm | $10(4)$ | $10(4)$ |
| Vertical $\beta^{*}$ | cm | $2(0.8)$ | $2(0.8)$ |
| Vertical beam-beam tuneshift |  | 0.015 | 0.03 |
| Laslett tuneshift |  | 0.06 | small |
| Distance from IP to 1 ${ }^{\text {st }}$ final focusing quad | m | $7(4.5)$ | 3.5 |
| Luminosity per IP | $10^{33} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ | $5.6(14.2)$ |  |

Table 7.6. MEIC design parameters for the full-acceptance detector. Values for the high-luminosity detector are given in parentheses.

The MEIC design calls for the construction of a green-field ion accelerator complex and two collider rings, one for electrons and the other for medium energy ions, as shown in figure 7.9. There are four crossing points of these figure-8 collider rings which will accommodate three detectors, at least two of which are available for medium-energy collisions, and the other for low-energy collisions with ions stored in a large booster. As presently envisaged, the two collider rings of identical circumferences are vertically stacked and the ion beams are transported into the plane of the electron ring via a vertical chicane, where horizontal crab crossings were used to collide the two beams at the collision points.


Figure 7.8. MEIC and its high-energy upgrade ELIC in CM energy-luminosity space.
The ion complex consists of ion sources, a 200 MeV SRF linac, a 3 GeV pre-booster and a large booster with energy up to 20 GeV . The ion beams are formed and accelerated in multiple stages in the low-energy ion complex, and are then filled into the collider ring for further acceleration to the colliding energy and stored for collision. A large figure-8 ring, also drawn in Fig. 7.9 (in grey), accommodates high-energy ion beams in a future energy upgrade. In that case, the compact medium-energy collider ring will act as another large booster. On the electron side, a 12 GeV upgraded CEBAF SRF linac will serve as a
full-energy injector into the electron collider ring, which could also be operated in a top-off mode in order to maintain high beam current. It is possible to continue the fixed target program for the CEBAF whenever there is a need, since each filling of the electron ring is very short.

The MEICs figure-8 shape in all
 rings is an optimal solution to preserve full polarization of light ion beams by avoiding spin resonances during acceleration in multiple booster and collider rings. It is also the only practical way to accelerate polarized deuterons and to arrange for longitudinal spin polarization at IP. The figure-8 layout allows for energy independence of the spin tune, as well as the transverse polarization of deuterons.

An essential component of every version of Jefferson Lab electron-ion collider design is an electron cooling facility, which is required for reducing ion beam transverse emittance and along with strong RF bunching, shortening the bunch length to 1 cm .

### 7.2.3 Ion Complex

Being primarily a lepton lab, Jefferson Lab does not have an ion complex at this time. This is usually considered a disadvantage to the Jefferson
Figure 7.9. Layout and side view of the MEIC and cross-section of tunnel. Lab electron-ion collider design effort, since a new ion complex is usually more expensive than a new electron complex. However, a green-field ion complex provides an excellent opportunity for applying new concepts and accelerator technologies which have been developed, tested and perfected over the last half century. Therefore, the MEICs ion complex could, in principle, be built to be far superior to the existing or legacy hadron facilities, thereby offsetting the relatively high project cost.

The main design goal of MEIC ion complex is to create and accelerate polarized or un-polarized ion beams with appropriate time, spatial and phase space structure matching the electron beam in order to implement the new luminosity concept. It is important to note that, while, on the one hand, the MEIC design requires bunch length and transverse emittances order of magnitude smaller than that of the conventional ion beams, on the other hand, due to a high bunch repetition rate, the MEIC ion bunch intensity is unusually low (at $4 \times 10^{9}$ ), approximately 50 times smaller than RHIC ion beam, thereby drastically easing the process of forming such ion beams and intensity dependent collective beam instabilities.

The MEIC ion complex is shown in figure 7.9 Its layout also characterizes the scheme of
ion beam acceleration and formation. The ions, coming out from the polarized or unpolarized sources, will be accelerated step-by-step to the colliding energy in the following major machine components: a 200 MeV SRF linac, a 3 GeV pre-booster, a 20 GeV large booster and finally a medium-energy collider ring of 20 to 60 GeV . All rings are in figure- 8 shape for the benefit of ion polarization. We will present a brief description on each component in the rest of this section. The pre-booster is also an accumulator ring, accepting and stacking ions ( 0.5 to 1 A average current) from a SRF linac in a multi-turn injection with assistance of a conventional DC electron cooling (except the case of $\mathrm{H}^{-} / \mathrm{D}^{-}$for which a phase space paint technique will be used). The accumulated ion beam in the pre-booster will become a coasting beam and will be re-bunched later in the medium-energy collider ring in order to decouple the RF frequencies in the linac and collider rings, as well as to suppress space charge tune-shift at low-energy stage.

## Ion Sources

The MEIC ion sources will rely on existing and mature technologies. We will have an Atomic Beam Polarized Ion Source (ABPIS) with Resonant Charge Exchange ionization for producing polarized light ions $\mathrm{H}^{+} / \mathrm{D}^{+}$and ${ }^{3} \mathrm{He}^{++}$. For unpolarized light to heavy ions, we will utilize Electron-Beam Ion Source (EBIS) which is current in operation at BNL. It is a realistic extrapolation, given future $R \& D$, that an ABPIS should be able to deliver 10 mA polarized $\mathrm{H}^{+} / \mathrm{D}^{+}$pulses at 5 Hz repetition frequency, over a 0.5 ms pulse length with a polarization better than $90 \%$. An EBIS, on the other, hand is expected to generate unpolarized ${ }^{208} \mathrm{~Pb}^{30+}$ pulses also at 5 Hz repetition rate and about 1.6 mA averaged current over a much shorter pulse length of 10 to $40 \mu \mathrm{~s}$. Alternatively, an Electron Cyclotron Resonance Source (ECR) can generate heavy ion beams with similar averaged currents, but 10 to 50 times longer pulse lengths, resulting in a factor of 10 or more pulse charges. In all of these instances, the present ion source technologies should be able to meet the requirement of the MEIC.

## Ion Linac

A technical design of an advanced SRF ion linac, originally developed at Argonne National Laboratory as a heavy-ion driver accelerator for Rare Isotope Beam Facility, has been adopted for the MEIC proposal. This $150-\mathrm{m}-\mathrm{long}$ linac, as shown in figure 7.10, is very effective in accelerating a wide variety of polarized and unpolarized ions from $\mathrm{H}(285 \mathrm{MeV})$ to ${ }^{208} \mathrm{~Pb}^{67+}(100 \mathrm{MeV} / \mathrm{u})$. Economic acceleration of lead ions up to $100 \mathrm{MeV} / \mathrm{u}$ requires a stripper with an optimal stripping energy of $13 \mathrm{MeV} / \mathrm{u}$. The stripping efficiency of ${ }^{208} \mathrm{~Pb}$ ion beam to the most abundant charge state $67+$ is $21 \%$.


Figure 7.10. Schematic drawing of MEIC SRF linac conceptual design.

## Pre-Booster/Accumulator Ring

The pre-booster ring, as shown in figure 7.11 is an essential component of the ion accelerator complex, which accepts beam pulses of any ions from the ion linac and, after accumulation and/or acceleration, transfers the beam to the subsequent large booster for further acceleration. The exact mechanisms of pre-booster operation depend on the ion species, relying on either combined longitudinal and transverse paint technique for $\mathrm{H}^{-} / \mathrm{D}^{-}$or conventional DC electron cooling for lead or other heavy metals during multiturn injection from the SRF linac. One important design consideration of the pre-booster is sufficiently high transition gamma, such that the ions never cross the transition energy during acceleration in order to prevent associated particle loss. In addition, the betatron motion working point should be carefully chosen such that the tune footprint does not cross low-order resonances.

| Length | Crossing angle | Max. beam size | $\gamma$ for 3 GeV particles | Transition $\gamma$ | Mom. compaction |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 234 m | 75 deg | 2.3 cm | 4.22 | 5 | 0.04 |

Table 7.7. Parameters for the pre-booster ring.


Figure 7.11. A figure-8 shaped pre-booster ring.

## Large Booster

The MEIC large booster shares the same tunnel as the electron and ion collider ring. It accelerates protons from 3 GeV to 12 to 20 GeV before sending them to the medium-energy collider ring. The extraction energy will be determined in the further design optimization. The boosters can handle all ion species. However, the energy will be affected by the ratio of charge and mass of the ion species. In principle, higher extraction energy is preferred. The key design requirements are that the ring must be also a figure- 8 shape, its magnetic lattice should be built by warm magnets and a crossing of the transition energy must be avoided. It should be pointed out that the large booster will be also used as a low-energy collider ring for collision energies in the region of 5 to 20 GeV per nucleon over only one detector. Special insertions such as an interaction region and an electron cooling facility must be inserted or added to meet such physics demand.

### 7.2.4 Collider Rings

Figure 7.12 shows a scaled layout of the electron and ion collider rings. When designing the optics of the electron and ion collider rings, the following geometric constraints must be taken into account:

- Figure- 8 shape, and four intersection points in two straights,
- Two short $(20 \mathrm{~m})$ straights in the middle of the two arcs for two Siberian snakes,
- A 60 m Universal Spin Rotator consisting of two solenoids and two sets of arc bending dipoles on each end of two electron arcs,
- Layouts of the interaction regions must match for both electron and ion rings,
- Footprints of the two collider rings must be very close so that they can be housed in one tunnel,
- The ion ring circumference must be equal to the big boosters length and be an integer multiple of the pre-boosters length for the purpose of RF matching.
The circumferences of the electron and ion rings are about 1340 m . The circumferences can be modified by adjusting length of straights, crossing angle and arc radii. The figure- 8 crossing angle is $60^{\circ}$. The electron and ion rings IPs coincide. The maximum separation of the electron and ion beam lines in the design is less than 4 m , which can be further reduced to be within the required limits once the optics design concept is finalized. The parameters of the electron ring and optics design are summarized in table 7.8,


Figure 7.12. Layout of the electron and ion collider rings.

| Arc's net bend | Crossing angle | Arc length | Arc avg. radius | straight length | circumference |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 240 deg | 60 deg | 405.75 m | 96.86 m | 264.46 m | 1340.41 m |

Table 7.8. Parameters for the collider ring.

### 7.2.5 Interaction Region

## Detector

The primary detector of the MEIC will be unique in its ability to provide almost full acceptance for the produced particles of electron-ion collisions. To accomplish this, a high
level of integration with the interaction region of the accelerator is required. The central detector will be built around a solenoid barrel, providing tracking, particle identification, and calorimetry for all particles, and two end-caps focusing on the detection of electrons and hadrons respectively. See section 7.3 for further discussion.

## Crab Crossing

With a 749 MHz bunch repetition rate for both colliding beams of MEIC, the bunch spacing is about 40 cm . A crab crossing of the colliding beams provides a simple way to separate quickly the two colliding beams near an IP to avoid undesired parasitic collisions. In the present MEIC IR design, the horizontal crabbing angle is 50 mrad . There are two ways currently under consideration to tilt the orientation of the electron or ion bunches in horizontal plane by a half crab crossing angle in order to restore head-on collisions. The first approach is placing crab cavities on each side of an IP. Such approach has been proved recently at KEK-B factory, which led to a record-high luminosity. It has been estimated that we need approximately 1.26 and 16.2 MV integrated transverse kicking voltage for 5 GeV electron and 60 GeV protons respectively. While a KEK-type squashed crab cavity should be readily adopted for the MEIC electron ring, the ion ring needs a set of such KEK crab cavities to achieve the design goal. At Jefferson Lab, a new type of crab cavity, which is more compact and promises much higher field, has been recently conceptually designed using transverse electromagnetic field (TEM), as another candidate of crab cavities for the MEIC. An alternative approach is dispersive crabbing, in which tilting of a bunch is achieved through purposely leaking the horizontal dispersion in the normal accelerating RF cavities.

## Interaction Region Design

As mentioned earlier, the two collider rings of MEIC are stacked vertically. In an early version of the IR design, the electron beam was vertically bent into a crab crossing, while the ion ring remains in a plane. Such design layout was abounded due to several problems: (i) bending electrons will generate excessive synchrotron radiation near an IP, which, consequently, interferes with the detector and degrades the background; (ii) the synchrotron radiation and quantum excitations in a beam extension area (betatron values are still very large) could enlarge the electron beam emittance by an order of magnitude; (iii) polarization decrease caused by vertical bend could be also very significant. The present MEIC IR design now requires the ions to undergo a vertical excursion to facilitate a horizontal crab crossing at an IP. For a 50 mrad crab crossing angle, the required bending field of the dipoles is quite modest for our ion energy range.

A typical magnet lattice layout of the MEIC interaction region is illustrated in figure 7.42. At a medium-energy region, the ion beams are modestly asymmetric in two transverse dimensions, as a result of balance of electron cooling and intra-beam scatterings. For instance, the emittance aspect ratio of a 60 GeV proton bunch is about 5. For such modestly flat beams, a final focusing quad doublet is a good choice.

For the MEIC IR design with a 2 cm or less $\beta^{*}$, chromatic aberration of the final focusing quads is one important issue that special attention must be paid. The chromaticity, defined as a ratio of betatron tune shift and momentum spread, could be as high as 110 per IR. A dedicated chromaticity compensation block, consisting of a set of sextupoles, will be inserted in the beam extension area on both sides of an IR to mitigate the problem. The initial studies indicate that, with proper values of these sextupoles, the chromaticity can be
reduced dramatically to single digits. Particle tracking simulations for dynamic aperture are currently underway.

### 7.2.6 Electron Cooling

Cooling of the ion beam is essential to achieve high luminosity in MEIC. At low energy, DC electron cooling is employed to help stacking of the ions in the pre-booster. At the collider ring, we rely on a concept of staged cooling of bunched ion beams of medium energies. Electron cooling is first called in the injection energy for reduction of the area that the ion beam occupies in the 6D phase space. After ions are accelerated to the collision energy, electron cooling will be utilized again for conditioning the beam to the design values. And most importantly, electron cooling will be continued during the collision mode to suppress the intra-beam scattering induced beam heating and emittance growth. Shortening the bunch length (down to 1 cm or less) that results from electron-cooling of the ion beam captured in a high voltage SRF field, in particular, it is critical for the high luminosity in MEIC, since it facilitates two important advances: an extreme focusing of the colliding beams and implementation of crab crossing at the IPs for achieving the highest bunch collision rate (up to 1.5 GHz ) and luminosity.

A schematic drawing of the MEIC ERL based electron cooler is shown in figure 7.13 , Two technologies, namely, energy recovery linac (ERL) and circulator ring, play critical roles to the success of this facility. A high-charge electron bunch from a photo-cathode is accelerated in a SRF ERL linac to required energy 10 to 50 MeV and then sent to a specially designed circulator cooler ring, with optics matching the cooling channel for cooling of a proton or ion bunch. The photo-injector and SRF linac ensure a high quality of the injected cooling bunch. An individual bunch circulates a large number of revolutions (up to a few hundred) in the ring before its quality is degraded by intra- and inter-beam scatterings, after which it returns to the same SRF linac for energy recovery. The recovered energy will be used for accelerating a new electron bunch. This circulator ring reduces the average current from a photo-cathode by a factor equal to the number of recirculation. Therefore, it provides a near-perfect solution for two bottlenecks of the facility: the high current and high power of the cooling electron beam. For example, a $3 \mathrm{~A}, 50 \mathrm{MV}$ (e.g. 150 MW of power) cooling beam can effectively be provided by $30 \mathrm{~mA}, 2 \mathrm{MV}$ (e.g 60 kW of active beam power) from the electron injector.

### 7.2.7 R\&D

For an advanced accelerator design like MEIC, there are many R\&D issues needed to be completed to solidify the design. We have identified a list of critical R\&D issues: electron cooling of the bunch ion beams at medium energy; crab crossing and crab cavity; polarization life time and spin tracking; beam-beam effects; non-linear collective beam effects and feedback systems; interaction region design and dynamic aperture, etc. The Jefferson Lab accelerator team and its collaborators are currently working on each of these issues. The details of the ongoing research are reported in a number of publications: overall design [1257, 1258], lattice design [1259, 1260], ion complex [1261, 1262, beam-beam simulations [1263, 1264], crab cavity [1265], electron cloud [1266], beam instabilities [1267], and others. For brevity, here we only highlight one topic from our R\&D list - beam-beam simulations.

Beam-beam interactions present a key limitation to collider performance, because they may lead to appreciable emittance growth of colliding beams and rapid reduction of lumi-


Figure 7.13. Schematic of electron cooling for the MEIC.
nosity. Such nonlinear collective beam effects can pose a significant design challenge when the machine parameters are pushed into a new regime. In order to lend credibility to the conceptual design, we use computer simulations to examine beam-beam instabilities, to optimize and explore limits of machine parameters.

A first phase of the beam-beam simulations of MEIC at Jefferson Lab, featuring a simplified model with linear transfer map, head-on collisions, and perfect chromaticity correction, has been already carried out for the current medium-energy configuration [1263, 1264, 1268] using the state-of-the-art beam collision code BeamBeam3D [1269]. These studies established that both designs were safely away from coherent beam-beam instabilities.

Furthermore, we use an evolutionary (genetic) algorithm [1270, 1271 to search for the optimal working point in the tune space, and demonstrated that such an approach is orders of magnitude more efficient than the simple tune scans [1272]. Figure 7.14 illustrates how the evolutionary algorithm successfully navigates the 4D betatron tune space ( 2 tunes for each beam) to find a (near-)optimal working point for which the luminosity exceeds the design luminosity by about $30 \%$.

### 7.2.8 Summary

The MEIC is the future of nuclear physics at Jefferson Lab. It is optimized to collide a wide variety of polarized light ions and unpolarized heavy ions with polarized electrons. It covers an energy range matched to the science program proposed by the Jefferson Lab nuclear physics community ( $\sim 4200 \mathrm{GeV}^{2}$ ), with luminosity exceeding $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. An upgrade path to higher energies $\left(250 \times 20 \mathrm{GeV}^{2}\right)$ has been developed and should provide luminosity of close to $10^{35} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$. The design is based on a figure- 8 ring for optimum polarization, and an ion beam with high repetition rate, small emittances and short bunch lengths.

We reported on the status of the design for the MEIC at Jefferson Lab. Our design is both mature, having addressed all the required aspects of the design in the various level of detail, and flexible, being able to accommodate revisions in design specifications and advances in accelerator $R \& D$. We have identified the critical accelerator R\&D topics for the MEIC, and are presently working on them.


Figure 7.14. MEIC beam-beam simulation with Evolutionary algorithm. Green line represents the design luminosity. The simulation locates a (near-)optimal working point within only 320 simulations (blue x ).

## Acknowledgment

We would like to thank members of the Jefferson Lab EIC nuclear science study group as well as the CEBAF user community for working with us on developing the MEIC design. In particular, we are grateful to Rolf Ent for coordinating the collaboration between the accelerator and nuclear physics groups, Alberto Accardi for generating Figure 7.14, Pawel Nadel-Turonski and Tanja Horn for their contributions on detector and interaction region design.

# 7.3 Kinematics and detector designs for the different EIC machine designs 

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### 7.3.1 Kinematics and Requirements for an EIC Detector

The physics program of an EIC imposes several challenges on the design of a detector, and more globally, the extended interaction region, as it spans a wide range in center-of-mass energy, different combinations of both beam energy and particle species, and several different physics processes. The various physics processes encompass inclusive measurements $\left(e p / A \rightarrow e^{\prime}+X\right)$, which require detection of the scattered lepton and/or the full scattered hadronic debris with high precision; semi-inclusive processes ( $e p / A \rightarrow e^{\prime}+h+X$ ), which require detection in coincidence with the scattered lepton of at least one (current or target region) hadron; and exclusive processes ( $e p / A \rightarrow e^{\prime}+N^{\prime} / A^{\prime}+\gamma / m$ ), which require detection of all particles in the reaction. The following figures in this section demonstrate the differences in particle kinematics of some representative examples of these reaction types, as well as differing beam energy combinations. For these plots, the directions of the beams are defined as for HERA at DESY: the hadron beam is in the positive z direction $\left(0^{\circ}\right)$ and the lepton beam is in the negative z-direction $\left(180^{\circ}\right)$. The upper panel of fig. 7.15 illustrates that the lower $\mathrm{Q}^{2}$ is, the closer the momentum of the scattered lepton is to the original lepton beam energy. For all lepton-hadron beam energy combinations (indicated by the panel in each of the plots), the scattered lepton goes in the direction of the original lepton beam for low $Q^{2}$ and more and more into a central detector acceptance for higher $Q^{2}$. For a fixed hadron beam energy the lepton scattering angle becomes smaller at a fixed $\mathrm{Q}^{2}$ with increasing lepton energy.

Fig. 7.16 shows the $\mathrm{x}-\mathrm{Q}^{2}$ plane for two different center-of-mass energies. In general, the correlation between $x$ and $Q^{2}$ for a collider environment is weaker than for fixed target experiments. Nonetheless, it becomes stronger for small scattering angles or corresponding small inelasticity $y$, and momentum and scattering angle resolution for the scattered lepton become an issue, at HERA roughly at $y=0.1$. To circumvent this problem, HERA reconstructed the lepton kinematics from the hadronic final state using the Jacquet-Blondel method [1273, 1274], and has reached successful measurements down to $y$ of 0.005 . The main reason why this hadronic method renders better resolution at low $y$ follows from the equation $y_{J B}=E-P_{z}^{\text {had }} / 2 E_{e}$, where $E-P_{z}^{\text {had }}$ is the sum over the energy minus the longitudinal momentum of all hadronic final-state particles and $E_{e}$ is the electron beam energy. This quantity has no degradation of resolution for $y<0.1$ as compared to the electron method, where $y_{e}=1-\left(1-\cos \theta_{e}\right) E_{e}^{\prime} / 2 E_{e}$. This is directly correlated to the relative resolutions for both quantities: $\Delta y_{J B} / y_{J B} \sim$ constant and $\Delta y_{e} / y_{e} \sim 1 / y_{e}$.

Typically, one can obtain for a given center-of-mass energy squared roughly a decade of $Q^{2}$ reach at fixed $x$ when using only an electron method to determine lepton kinematics, and roughly two decades when including the hadronic method. If only using the electron method, one can increase the range in accessible $Q^{2}$ by lowering the center-of-mass energy, as can be seen from comparing the two panels of fig. 7.16. This may become relevant for some semi-inclusive and exclusive processes. The advantages and disadvantages of this solution are discussed in the two machine-specific detector sections of this section.

In general, one would like to access as large a range in $Q^{2}$ at fixed $x$ as possible for a given beam energy combination, and reach as low $y_{J B}$ as possible. This requirement


Figure 7.15. $\mathrm{Q}^{2}$ vs. momentum (upper panel) and $\mathrm{Q}^{2}$ vs. scattering angle (lower panel) of the scattered lepton in the laboratory frame. The following cuts have been applied in both figures: $\mathrm{Q}^{2}>0.1 \mathrm{GeV}^{2}, 0.01<\mathrm{y}<0.95$. The lepton-hadron beam energy combinations are indicated by the panel in each individual plots
directly implies two important considerations for the detector design:

- good hadronic coverage in the forward direction
- low noise and/or good noise suppression algorithms in the hadronic calorimeter to allow for hadron detection down to 0.5 GeV . More detailed detector simulations are needed to confirm these requirements.


Figure 7.16. The $\mathrm{x}-\mathrm{Q}^{2}$ plane for center-of-mass energy 45 GeV (left) and 140 GeV (right). The black lines indicate different $y$-cuts placed on the scattered lepton kinematics.

It is important to point out that the reconstruction of the event kinematics from the hadronic final state is also important in suppressing events with radiation of a real or virtual photon from the incoming or outgoing lepton (radiative corrections); for details please see section 7.3.2.

One should keep in mind that there are additional complications at low $y$ for the measurement of asymmetries and/or polarized cross sections, to for example extract the helicitydependent parton distributions. A depolarization factor, defined in [1275] as:

$$
\begin{equation*}
D=\frac{y\left[\left(1+\gamma^{2} y / 2\right)(2-y)-2 y^{2} m_{e}^{2} / Q^{2}\right]}{y^{2}\left(1-2 m_{e}^{2} / Q^{2}\right)\left(1+\gamma^{2}\right)+2(1+R)\left(1-y-\gamma^{2} y^{2} / 4\right)} \tag{7.1}
\end{equation*}
$$

is needed to correct the measured helicity-dependent asymmetries $\left(A_{\|}\right)$. The depolarization factor corrects for the polarization transfer from the lepton to the virtual photon, and is small at low $y$. This reduces the effective polarized luminosity and increases the uncertainties of the measured polarized quantities at low y $\left(\delta A_{1}=\delta A_{\|} / D\right)$. Therefore, the $x-Q^{2}$-plane of precision polarized cross section measurements will be reduced as compared to unpolarized ones, for fixed center-of-mass energy.

Fig. 7.17 shows the momentum versus scattering angle distributions in the laboratory frame for pions originating from semi-inclusive reactions, for different lepton and proton beam energy combinations. For lower lepton energies, pions are scattered more in the forward (ion) direction. For fixed low lepton energy of 5 GeV , this pattern remains more or less constant as a function of proton energy. With increasing lepton beam energy, the hadrons increasingly populate the central region of the detector, and at the highest lepton energies, hadrons are even largely produced going backward (i.e. in the lepton beam direction). The kinematic distributions for kaons and protons, applying the same cuts as for pions, are essentially identical to those of the pions. The distributions for semi-inclusive events in electron nucleus collisions may be slightly altered due to nuclear modification effects, but the global features will remain.


Figure 7.17. Momentum vs. scattering angle in the laboratory frames for pions from non-exclusive reactions. The following cuts have been applied: $\mathrm{Q}^{2}>1 \mathrm{GeV}^{2}, 0.01<\mathrm{y}<0.95$ and $0.1<\mathrm{z}<0.9$

Fig. 7.17 also indicates a shift of the momentum range of pions towards higher momenta in the central-angle region for higher lepton energy, to typical momenta of about $10 \mathrm{GeV} / \mathrm{c}$, which has implications for the required particle identification (PID). To be able to identify the different hadron types over a wide momentum and angular range an EIC detector needs to have detectors capable of good PID in the forward, central and backward direction. For the higher hadron momenta, typically in the forward ion direction and also in the backward direction for higher lepton beam energies, the most viable detector technology is a RingImaging Cherenkov (RICH) detector with dual-radiators. In the central detector region a combination of high resolution time-of-flight (ToF) detectors (preferentially with timing resolutions $\delta \mathrm{t} \sim 10 \mathrm{ps}$ ), a DIRC, or a proximity focusing Aerogel RICH may be adequate detector technologies.

For certain kinematics, the hadrons (both charged and neutral) will be produced in the backward ion direction (see fig. 7.18) and need to be disentangled from the scattered leptons. The kinematic region in rapidity $\eta$, over which hadrons and photons need to be suppressed with respect to electrons, shifts to more negative rapidity with increasing center-of-mass energy. This can be cross-correlated with the angular and momentum patterns for scattered leptons of fig. 7.15] For the lower center-of-mass combination, electron, photon and charged hadron rates are roughly comparable at $1 \mathrm{GeV} / \mathrm{c}$ total momentum and $\eta=$ -3 . For the higher center-of-mass energy, electron rates are a factor of $10-100$ smaller than photon and charged hadron rates, and comparable again at a $10 \mathrm{GeV} / \mathrm{c}$ total momentum.

This adds another requirement to the detector: good electron identification. The kinematic region in rapidity $\eta$ over which hadrons and also photons need to be suppressed, typically by a factor of $10-100$, shifts to more negative rapidity with increasing center-
of-mass energy. Measuring the ratio of the lepton energy and momentum, $\mathrm{E}_{e}^{\prime} / \mathrm{p}_{e}^{\prime}$, typically gives a reduction factor of $\sim 100$ for hadrons. This requires the availability of both tracking detectors (to determine momentum) and electromagnetic calorimetry (to determine energy) over the same rapidity coverage. This availability also immediately suppresses the misidentification of photons in the lepton sample, by requiring that a track must point to the electromagnetic cluster. Of course, the availability of good tracking detectors over similar coverage as electromagnetic calorimetry similarly aids in $y$ resolution at low y from a lepton method only (see earlier), as the angular as well as the momentum resolution for trackers are much better than for electromagnetic calorimeters. The hadron suppression can be further improved by adding a Cherenkov detector to the electromagnetic calorimetry. Combining the electromagnetic calorimeter response and the response of Cherenkov detectors may especially help in the region of low-momentum scattered leptons, about 1 $\mathrm{GeV} / \mathrm{c}$. Other detector technologies, such as transition radiation detectors, may provide another factor 100 hadron suppression for lepton momenta greater than $4 \mathrm{GeV} / \mathrm{c}$.

An additional advantage of a collider detector over a fixed target experiment is the large coverage in transverse momentum. This is especially important for measurements linking the perturbative high-transverse momentum $p_{T}$ region to the region of small transverse momentum, $p_{T} \sim \Lambda_{Q C D}$, where single-spin asymmetries as functions of $p_{T}, x, Q^{2}, z$ and $\phi$ are the prime observable to extract TMDs - Transverse Momentum Dependent Parton Distributions (see chapter (2), like the Sivers function. Fig. 7.19 shows the coverage in hadron $\mathrm{p}_{T}$ measured with respect to the virtual photon vs. $z=E_{h} / \nu$ assuming an angular acceptance of a detector $0.5^{\circ}<\theta<179.5^{\circ}$. One can see that for all beam energy combinations a large range in transverse momentum is achievable. In general, such physics does not drive the most forward (or backward) detector requirements, leaving ample phase space in transverse momentum with respect to the virtual-photon direction - typically more central.

There is specific interest in detecting events with heavy quarks (charm or bottom). To measure the inclusive structure functions, $\mathrm{F}_{2}^{c}, \mathrm{~F}_{L}^{c}$, and $\mathrm{F}_{2}^{B}$ for heavy quarks, it is sufficient to tag the charm and the bottom quark content via the detection of additional leptons (electron, positron, muons) to the scattered lepton. The leptons from charmed mesons can be identified via a displaced vertex of the second lepton ( $<\tau>\sim 150 \mu \mathrm{~m}$ ). This can be achieved by integrating a high-resolution vertex detector into the detector design. For measurements of the charmed (bottom) fragmentation functions, or to study medium modifications of heavy quarks in the nuclear environment, at least one of the charmed (bottom) mesons must be completely reconstructed to have access to the kinematics of the parton. This requires, in addition to measuring the displaced vertex, good particle identification to reconstruct the meson via its hadronic decay products, e.g. $D_{0} \rightarrow K^{ \pm}+\pi^{\mp}$.

Fig. 7.20 (upper panel) shows the momentum versus scattering angle distributions for pions following from an exclusive reaction with a $\rho^{0}$ vector meson production $\left(Q^{2}>1.0\right.$ $\mathrm{GeV}^{2}$ ), in the laboratory frame and for different beam energy combinations. As in fig. 7.17, two familiar patterns arise. For increasing lepton beam energy, the pion distribution goes from being more peaked in the forward-angle direction to a distribution with both a peak in the forward and backward ion direction, and the momentum in the forwardion direction is slightly reduced. Most of the forward-ion direction pions in fig. 7.20 are correlated with lower- $Q^{2}$ processes, though possibly of less interest for these processes. If one would use a $Q^{2}>10 \mathrm{GeV}^{2}$ cutoff in these exclusive processes, only a peak in the backward-ion direction would remain and in that sense, lower lepton energies correspond to lower hadron momenta on average and reduced particle identification requirements. The distributions for kaons from exclusive $\phi$-mesons production as well as for muons/electrons


Figure 7.18. The number of photons and hadrons as well as the number of scattered leptons in a rapidity bin vs momentum having 5 GeV leptons colliding with 100 GeV protons and 20 GeV leptons colliding with 250 GeV protons. No kinematic cuts are applied.


Figure 7.19. Transverse momentum vs. z for pions applying the following cuts $\mathrm{Q}^{2}>1 \mathrm{GeV}^{2}, 0.01<$ $\mathrm{y}<0.95,0.5^{\circ}<\theta<179.5^{\circ}$ and $\mathrm{p}>1 \mathrm{GeV}$. A momentum cut is applied to simulate the threshold of potential particle-identification-detectors.
from exclusive $J / \psi$ production look very similar, see lower panel of fig. 7.20. The most challenging constraints on the detector design for exclusive reactions compared to semiinclusive reactions is, however, not given by the hadrons originating from vector mesons, but from the detection of the exclusive hadronic state remaining.

As one specific example of an exclusive reaction, deeply virtual compton scattering (DVCS) was chosen, fig. 7.21 (top) shows the energy versus scattering angle distributions of photons in the laboratory frame, for different beam energy combinations. A cut of $\mathrm{Q}^{2}>$ $1 \mathrm{GeV}^{2}$ is assumed, although larger values of $\mathrm{Q}^{2}$ may be required. Lower lepton energies show a more symmetric distribution, and higher lepton energies are more backward-ion angle peaked. The distributions show relatively homogeneous distributions of the DVCS photons from forward to backward, with a small preference for the backward direction. The latter is true for all lepton-hadron beam energy combination.

Fig. 7.21 (bottom) correlates the distribution of the photon angle and the electron scattering angle in the laboratory frame, for different beam-energy combinations. With increasing lepton beam energy, the photon and scattered lepton tend towards the same detector hemisphere. Following fig. 7.21 (top), electromagnetic calorimetry is required over the entire rapidity range of the detector. Fig. 7.21 (bottom) illustrates that tracking and electromagnetic calorimetry capabilities covering similar rapidity range will greatly aid the separation of the photon and lepton, reducing a difficulty encountered by the ZEUS collaboration in their DVCS event reconstruction.

For exclusive reactions in general, with DVCS as the example above, it is extremely important to ensure that the remaining nucleon (or the nucleus) remains intact during the


Figure 7.20. Upper Panel: Momentum vs. scattering angle in the laboratory frames for pions following from exclusive $\rho^{0}$ vector meson production. The following cuts are applied: $\mathrm{Q}^{2}>1.0$ $\mathrm{GeV}^{2}, 0.01<\mathrm{y}<0.95$.
Lower Panel: Momentum vs. scattering angle in the laboratory frames for muons following from exclusive $\mathrm{J} / \psi$ vector meson production. No cuts on $\mathrm{Q}^{2}$ have been applied as a hard scale for the process is given by the $\mathrm{J} / \psi$ mass.


Figure 7.21. Upper panel: Energy vs. scattering angle in the laboratory frame for photons from DVCS. The following cuts have been applied: $\mathrm{Q}^{2}>1.0 \mathrm{GeV}^{2}, 0.01<\mathrm{y}<0.95$ and $\mathrm{E}_{\gamma}>1$. GeV . Lower Panel: The scattering angle in the laboratory frame of the photon vs. that of the scattered lepton for DVCS events. The following cuts have been applied: $\mathrm{Q}^{2}>1.0 \mathrm{GeV}^{2}, 0.01<\mathrm{y}<0.95$ and $\mathrm{E}_{\gamma}>1 . \mathrm{GeV}$
scattering process. Hence, one has to ensure exclusivity by measuring all products. Fig. 7.22 illustrates the kinematic requirements for the DVCS case, showing the scattered proton momentum versus its scattering angle for three different beam energy combinations. In general, for exclusive reactions one wishes to map the four-momentum transfer (or Mandelstam variable) t to the hadronic system, and then obtain an image by a Fourier transform, at relatively low t of up to $1-2 \mathrm{GeV}$. The angle of the recoiling hadronic system is directly correlated with $t$ and the proton energy $E_{p}$, as $\sqrt{t} / E_{p}$. As can be seen in fig. 7.22, the proton scattering angle requirements indeed linearly (and inversely) scale with proton energy.

Even at a proton energy of 50 GeV , the proton scattering angles only range to about $1-2^{\circ}$. At proton energies of 250 GeV , this number is reduced to one fifth. In all cases, one obtains small to extremely small scattering angles, extending to or completely within the $0.5^{\circ}$ angular detector cutoff often used above. Because of this, the detection of these protons, or more general recoil baryons, is extremely dependent on the exact interaction region design and will therefore be discussed in more detail in the machine-dependent part of this chapter.


Figure 7.22. Scattered proton momentum vs. scattering angle in the laboratory frames for DVCS events with different beam energy combinations. The following cuts have been applied: $1 \mathrm{GeV}^{2}<$ $\mathrm{Q}^{2}<100 \mathrm{GeV}^{2}, 10^{-5}<\mathrm{x}<0.7$ and $0<\mathrm{t}<2 \mathrm{GeV}^{2}$.

Detection of the intact nucleus following an exclusive reaction in eA collisions is even more complicated. The binding energy in heavy nuclei is of the order 8 MeV per nucleon. In general, the smallest measurable outgoing angle of heavy scattered or fragmented nuclei, $\theta_{\text {min }}$, is limited by the beam angular divergence and the requirement to have a $\sim 10 \sigma$ clearance of any detector element (often 'Roman pots') from the beam. For a beam divergence of say 0.1 mrad and an ion beam of $100 \mathrm{GeV} / \mathrm{u}$, the transverse momentum required in the nuclear breakup to be beyond the so-called machine 'beam-stay-clear' area of $\sim 10 \sigma$ is 100

MeV , well beyond the 8 MeV (or so) needed for a single nucleon. This would assume that the transverse momentum is equal to the excitation energy of the nucleus.

The diffractive slope at $\mathrm{t}=0$ depends on the size of the nucleus. Fig. 5.88 shows, for small $t \sim 1 / R_{A}^{2}$, a very steep t dependence, $\sim \exp \left(-t R_{A}^{2} / 3\right)$, and then several diffractive $\operatorname{minima}\left(R_{A}=(1.12 \mathrm{fm}) A^{1 / 3}-(0.86 \mathrm{fm}) A^{-1 / 3}\right.$, for details see [1276]). The incoherent background starts to dominate at $t$ values at which the coherent cross section has fallen to $1 / e$. These $t$ values can be estimated by $\exp \left(-|t| B_{0} A^{2 / 3}\right)=1 / A$, with $B_{0}=(1.12 f m)^{2 / 3}$. These values of $t$ are much smaller than the $t$ value corresponding to the first minimum in the coherent cross section and the $t$-values corresponding to the smallest measurable outgoing angle of scattered heavy nuclei. Therefore the strategy to ensure exclusive production on a nucleus is to veto nuclear breakup, by detecting the neutrons from incoherent events.

Another possibility can be to require a rapidity gap between the hadron beam and the produced jet, (vector) meson or real photon (where all events represent the sum of elastic and incoherent events). The left panel of fig. 7.23 shows the rapidity distribution of the most forward particle in deep-inelastic scattering (blue filled distribution) and diffractive events (unfilled histogram), respectively, for a 5 GeV electron and a 100 GeV proton beam energy combination. The 100 GeV is here chosen to mimic the $100 \mathrm{GeV} / \mathrm{u}$ ion beam. The right panel of fig. 7.23 shows the efficiency and purity for diffractive events to DIS events (1:1) as function of rapidity, varying the lepton beam energy while keeping the hadron beam energy fixed. If one requires 4 units of rapidity between the hadron beam and a produced jet, vector meson or real photon, an efficiency of above $60 \%$ and a purity close to $100 \%$ for diffractive events would be obtained. A detector with wide rapidity coverage is essential for


Figure 7.23. Left: Rapidity distribution of DIS and diffractive events for the most forward particle (MFP) in the event. Right: Efficiency and Purity for diffractive events with respect to DIS events (1:1) as a function of the detector rapidity coverage and the center-of-mass energy.
such events.

### 7.3.2 Radiative Corrections

The radiation of real and virtual photons leads to large additional contributions to the observable cross section of electron scattering at high energies. Precision measurements of the nucleon structure require a good understanding of these radiative corrections. For neutral-current lepton nucleon scattering, a gauge-invariant classification into leptonic, hadronic and interference contributions can be obtained from Feynman diagrams. The Feynman diagrams for leptonic corrections are shown in fig. 7.24, Leptonic corrections dominate and strongly affect the experimental determination of kinematic variables.

Usually, the cross section is measured as a function of $Q^{2}$ and Bjorken-x, $x_{B}$, defined as

$$
\begin{equation*}
Q^{2}=-\left(l-l^{\prime}\right)^{2}, \quad x_{B}=\frac{Q^{2}}{2 P \cdot\left(l-l^{\prime}\right)}, \tag{7.2}
\end{equation*}
$$

where $l$ and $l^{\prime}$ denote the 4 -momenta of the incoming and outgoing lepton, respectively, and $P$ is the 4 momentum of the incoming nucleon. The true values of these variables seen by the nucleon when a photon with 4 -momentum $k$ is radiated are, however, given by (see fig.)

$$
\begin{equation*}
\tilde{Q}^{2}=-\left(l-l^{\prime}-k\right)^{2}, \quad \tilde{x}_{B}=\frac{\tilde{Q}^{2}}{2 P \cdot\left(l-l^{\prime}-k\right)} . \tag{7.3}
\end{equation*}
$$

If the photon momentum is large and balancing the transverse momentum of the scattered lepton, $\tilde{Q}^{2}$ can be shifted to small values, leading to an enhancement of the radiative corrections. This effect is similar to the radiative tail of a resonance.


Kinematics of leptonic radiation.


Figure 7.24. Feynman diagrams for leptonic radiation in lepton-quark scattering.
The effect of radiation of photons from the lepton can be described with the help of radiator functions $\tilde{R}_{i}\left(l, l^{\prime}, k\right)$. There is one $\tilde{R}_{i}$ for every structure function $F_{i}, i=2, L$. The radiator functions comprise both real radiation from the initial and the final state as well as the contribution from vertex and self-energy diagrams. Using $\tilde{x}_{B}$ and $\tilde{Q}^{2}$ from equation (7.3) to parametrize the integration over the phase space of emitted photons, one can express the observed structure functions as convolutions,

$$
\begin{equation*}
F_{i}^{\mathrm{obs}}\left(x_{B}, Q^{2}\right)=\int \mathrm{d} \tilde{x}_{B} \mathrm{~d} \tilde{Q}^{2} R_{i}\left(x_{B}, Q^{2}, \tilde{x}_{B}, \tilde{Q}^{2}\right) F_{i}^{\mathrm{true}}\left(\tilde{x}_{B}, \tilde{Q}^{2}\right) \tag{7.4}
\end{equation*}
$$

The integration limits are determined by the energy allowed for the radiated photon which, in the photon-nucleon center-of-mass frame, is given by

$$
\begin{equation*}
E_{\gamma}^{\max }=\sqrt{\frac{1-x_{B}}{x_{B}} Q^{2}} \tag{7.5}
\end{equation*}
$$

Radiative corrections are, therefore, large at large $Q^{2}$ and small $x_{B}$. In contrast, at small $Q^{2}$ and large $x_{B}$, the phase space for photon emission is restricted and negative virtual corrections dominate.

From equation (7.4) it is obvious that the determination of the true structure functions $F_{i}^{\text {true }}\left(\tilde{x}_{B}, \tilde{Q}^{2}\right)$ requires unfolding, a procedure which is in general only possible in an iterative way and with reasonably chosen assumptions about the starting values. Moreover, the observed structure functions depend on the way in which the kinematic variables are measured. For example, if the momentum of the hadronic final state, $p_{X}$, could be measured, $\tilde{x}_{B}$ and $\tilde{Q}^{2}$ would be known. In practice this will be difficult to achieve; however, any information about the hadronic final state could contribute to a narrowing down of the phase space available for photon emission, thereby reducing the size of radiative corrections.

The radiator functions are dominated by peaks in the angular distribution for the collinear radiation of photons from the initial state (ISR) or from the final state (FSR). At high energies, it is a good approximation to assume that photon radiation can be described by a simple rescaling of the lepton momentum, $l \rightarrow z l$ for ISR and $l^{\prime} \rightarrow l^{\prime} / z$ for FSR. The radiator function in the collinear approximation takes the simple, universal form

$$
\begin{equation*}
R_{\text {coll }}=\frac{\alpha}{2 \pi} \log \frac{Q^{2}}{m_{e}^{2}}\left(\frac{1+z^{2}}{1-z}\right)_{+} \tag{7.6}
\end{equation*}
$$

so that the cross section is obtained from

$$
\begin{equation*}
\mathrm{d} \sigma_{\mathrm{ISR}}=\int \frac{\mathrm{d} z}{z} R_{\mathrm{coll}}(z) \mathrm{d} \sigma_{\mathrm{Born}}\left(l^{\mu} \rightarrow z l^{\mu}\right) \tag{7.7}
\end{equation*}
$$

(and similarly for FSR). The potentially large $\operatorname{logarithm} \log Q^{2} / m_{e}^{2}$ may reach the order of $10 \%$ at large $Q^{2}$.

As an example, we show numerical results for electron proton scattering at two typical sets of beam energies: $E_{e}=5 \mathrm{GeV}$ with $E_{p}=50 \mathrm{GeV}$ (left panel of fig. 7.25) and $E_{e}=30$ GeV with $E_{p}=325 \mathrm{GeV}$ (right panel). The figures show the correction factor

$$
\begin{equation*}
r_{c}(y)=\frac{\mathrm{d} \sigma /\left.\mathrm{d} y\right|_{O(\alpha)}}{\mathrm{d} \sigma /\left.\mathrm{d} y\right|_{B o r n}}-1 \tag{7.8}
\end{equation*}
$$

where $y=Q^{2} / Q_{\max }^{2}, Q_{\max }^{2}=x_{B} S, S=2 l \cdot P$. The different curves correspond to different ranges of $x_{B}$ : at the lower center-of-mass energy (left panel of fig. 7.25, from the bottom up): $0.1<x_{B}<0.4,10^{-2}<x_{B}<10^{-1}$ and $10^{-3}<x_{B}<10^{-2}$; at the higher center-ofmass energy (right panel, again from the bottom up): $0.1<x_{B}<0.4,10^{-2}<x_{B}<10^{-1}$, $10^{-3}<x_{B}<10^{-2}, 10^{-4}<x_{B}<10^{-3}$, and $10^{-5}<x_{B}<10^{-4}$. The general features following from the preceding discussion are clearly visible: corrections are large at large $y$ and small $x_{B}$, while corrections become negative at large $x_{B}$ and small $y$.

Lacking a full Monte Carlo event simulation for scattering with heavy nuclei at present, we have studied the influence of a simple cut on the invariant mass of the hadronic final state. Imposing the condition $W_{\text {had }}>1.4 \mathrm{GeV}$ would remove the elastic tail and the contribution


Figure 7.25. $y$-dependence of the leptonic radiative correction factor for electron proton scattering with different beam energies and in different $x_{B}$ ranges. Left: $E_{e}=5 \mathrm{GeV}, E_{p}=30 \mathrm{GeV}$ and the curves from the bottom up correspond to $0.1<x_{B}<0.4,10^{-2}<x_{B}<10^{-1}, 10^{-3}<x_{B}<10^{-2}$; Right: $E_{e}=30 \mathrm{GeV}, E_{p}=325 \mathrm{GeV}$ and $0.1<x_{B}<0.4,10^{-2}<x_{B}<10^{-1}, 10^{-3}<x_{B}<10^{-2}$, $10^{-4}<x_{B}<10^{-3}, 10^{-5}<x_{B}<10^{-4}$ (full and dashed lines alternating for better visibility).


Figure 7.26. Influence of a cut on the mass of the hadronic final state on the leptonic radiative correction factor for a proton target in different $x_{B}$ ranges and beam energies as indicated in the figures. Dashed curves are without a cut, full curves are obtained after a cut of $W_{\text {had }}>1.4 \mathrm{GeV}$.
from low-lying resonances. A similar effect can be achieved cutting on $E-p_{z}$ from the Jacquet-Blondel method. The effect of such a naive cut is shown in fig. 7.26. The reduction of the radiative corrections is considerable at largest $y$ and at small $x_{B}$, but probably not yet sufficient at larger values of $x_{B}$. From similar studies for electron-nucleus scattering at HERA [1277, 1278, 1274, one can expect to obtain a much stronger reduction of radiative corrections, if more refined prescriptions for the measurement of kinematic variables are found.


Figure 7.27. Left: Radiative corrections for electron scattering off a Au nucleus at $5 \times 130 \mathrm{GeV}^{2}$ beam energies, $10^{-3}<x_{B}<10^{-2}, Q^{2}>1 \mathrm{GeV}^{2}, W_{\text {had }}>1.4 \mathrm{GeV}$ with different models for nuclear PDFs: EPS09 (full curve), EPS08 (dash-dotted line), EKS98 (dashed line) and HKN (dotted line). Right: Radiative corrections for different nuclei with CTEQ61M PDFs modified by the EPS09 prescription. Beam energies and kinematic range as in the left figure. From the bottom up: proton, ${ }^{4} \mathrm{He},{ }^{56} \mathrm{Fe}$, ${ }^{197} \mathrm{Au}$.

Since the determination of the true structure functions requires an iterative unfolding procedure, it is important to show that the radiative corrections do not depend too strongly on the assumed input structure functions. In fig. 7.27a we show the correction factor $r_{c}(y)$ as defined above for the case of electron scattering off an ${ }^{197} \mathrm{Au}$ nucleus, assuming different parameterizations of parton distribution functions corrected for nuclear effects, as available in the literature [38, 828, 1279, 40]. Although differences at the level of $10 \%$ are visible, one can still observe a similar overall behavior of radiative corrections. Finally, in fig. 7.27b, we show results for scattering off different nuclei, again supporting the assumption that a common unfolding procedure would allow one to obtain the true structure functions.

Corrections due to the emission of photons from the hadrons, or quarks in the deep inelastic regime, require a careful separation into contributions which should be considered as a part of the hadron structure (leading to an electromagnetic contribution to scaling violations [1280]) and contributions which can, in principle, be related to the observation of direct photons radiated from quarks. The interference of radiation from the lepton and the quark is small [1277]. In certain phase space regions one may expect higher than one-photon corrections to be important. For example, soft-photon exponentiation will be necessary at small $y$ and large $x_{B}$. The procedure is well-known and straightforward. Finally, multi-
photon radiation may become important at large $y$ and small $x_{B}$. In this case, the collinear approximation is sufficient to reach a precision at the level of one percent [1281].

### 7.3.3 Detector Design for eRHIC

The BNL design of an EIC allows for collisions at three interaction regions: one at IP-12 with a new dedicated EIC detector, and at IP-6 and IP-8 with the current RHIC detectors STAR and PHENIX. In the following, first the design considerations for a dedicated EIC detector are described and then the capabilities of PHENIX and STAR for ep / eA collisions are discussed.

## A dedicated EIC detector

Combining all the requirements described in section 7.3 .1 and in the physics chapters before, a schematic view of the emerging dedicated eRHIC detector is shown in fig. 7.28, As already discussed, it is important to have equal rapidity coverage for tracking and


Figure 7.28. A schematic view of a dedicated EIC detector. Details of the GEANT-3 model can be found at https://wiki.bnl.gov/eic/index.php/Detector_Design.
electromagnetic calorimetry. This will provide good electron identification and give better momentum and angular resolutions at low inelasticity $y$ than with an electro-magnetic calorimeter alone.

The significant progress in the last decade in the development of Monolithic Active Pixel Sensors (MAPS), in which the active detector, analog signal shaping, and digital conversion take place in a single silicon chip (i.e. on a single substrate; see [1282 and references therein), provides a unique opportunity for a $\mu$-vertex detector for an eRHIC detector. These devices, built using CMOS technology, use an epitaxial layer as the active sensing element. Ionization deposited in the epitaxial layer is collected by $\mathrm{N}+$ wells embedded in
the epitaxial layer. The "pixel" pitch is determined by the location of the N wells so there is no need for actual segmentation of the detector as is done with traditional hybrid pixel detectors. As a result, CMOS pixel detectors can be built with high segmentation, limited primarily by the space required for additional shaping and digital conversion elements. The key advantage of CMOS MAPS detectors is the reduced material required for the detector and the (on substrate) on-detector electronics. Such detectors have been fabricated and extensively tested (see e.g. [1283]) with thicknesses of about $50 \mu \mathrm{~m}$, corresponding to $0.05 \%$ of a radiation length.

For tracking at larger radii, there are several possibilities which need to be investigated first through Monte Carlo studies for position resolution and material budget, and later through R\&D and building prototypes. The two most prominent options for the barrel tracker are a TPC and a cylindrical GEM-Tracker. For large radii, forward tracking GEMTrackers are the most likely option. The projected rates for a luminosity of $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$ range, depending on the center-of-mass energy, between 300 and 600 kHz , with an average of 6 to 8 charged tracks per event. These numbers do not impose strong constraints on the technology for a tracker.

Due to the momentum range to be covered, the only solution for PID in the forward direction is a dual radiator RICH, combining either Aerogel with a gas radiator like $\mathrm{C}_{4} \mathrm{~F}_{10}$ or $\mathrm{C}_{4} \mathrm{~F}_{8} \mathrm{O}$ if $\mathrm{C}_{4} \mathrm{~F}_{10}$ is no longer available, or combining the gas radiator with a liquid radiator like $\mathrm{C}_{6} \mathrm{~F}_{14}$.

In the barrel part of the detector several solutions are possible, as the momenta of the majority of the hadrons to be identified are between 0.5 GeV and 5 GeV . The technologies available in this momentum range are high resolution ToF detectors ( $\mathrm{t} \sim 10 \mathrm{ps}$ ), a DIRC or a proximity focusing Aerogel RICH.

For the electromagnetic calorimetry in the forward and backward direction, a solution based on $\mathrm{PbWO}_{4}$ crystals would be optimal. The advantages of such a calorimeter would be a small Molière radius of 2 cm and a factor of two better energy resolution and higher radiation hardness than, for example, lead-glass. To increase the separation of photons and $\pi^{0}$ s to high momenta and to improve the matching of charged tracks to the electromagnetic cluster, it would be an advantage to add, in front of all calorimetry, a high resolution pre-shower. We follow for the barrel part of the detector the concept of very compact electromagnetic calorimetry (CEMCal). A key feature is to have at least one preshower layer with 1-2 radiation lengths of tungsten and silicon strip layers (possibly with two spatial projections) to allow separation of single photons from $\pi^{0}$ to up $p_{T} \approx 50 \mathrm{GeV}$, as well as enhanced electron-identification. A straw-man design could have silicon strips with $\Delta \eta=0.0005$ and $\Delta \phi=0.1$. The back section for full electromagnetic energy capture could be, for cost effectiveness and good uniformity, an accordion Lead-Scintillator Design, which would provide gain uniformity and the ability to calibrate the device. A tungsten- and silicon-strip-based pre-shower would also be a good solution for the forward and backward electromagnetic calorimetry.

To achieve the physics program as described in earlier sections, it is extremely important to integrate the detector design into the interaction region design of the collider. As already described, particularly challenging is the detection of forward-going scattered protons from exclusive reactions, as well as of decay neutrons from the breakup of heavy ions in nondiffractive reactions. Previous experience of electron colliders (SLAC, KEK B-factories) and HERA, an electron-proton collider, indicated difficulties with synchrotron radiation coming from bending the electron beam close to the interaction region (IR). The newest large improvements in luminosity at KEK in Japan, by introducing crab cavities, show
that colliding heavy ions or protons with electrons could be obtained without bending the electrons close to the IR, but that it is possible to use the crossing angle between the two beams without losing luminosity. This is the path chosen in the eRHIC design: a 10 mrad crossing angle between the protons or heavy ions during collisions with electrons. This choice removes potential problems for the detector induced by synchrotron radiation. To obtain luminosities higher than $10^{34} \mathrm{~cm}^{-2} \mathrm{~s}^{-1}$, very strong focusing close to the IR is required to have the smallest beam sizes at the interaction point. A small beam size is only possible if the beam emittance is also very small. The focusing triplets are 4.5 meters away from the interaction point (IP). The strong focusing quadrupoles induce very large chromaticities. The current eRHIC design has its highest values of the amplitude betatron functions of the same size as the present operating conditions of the RHIC collider. In addition the design allows a correction of the first, second and third order chromaticities by using sextupoles at the triplets as well as 180 degrees away from the quadrupoles source (as shown in fig. 7.29).


Figure 7.29. The Beta-function along the eRHIC hadron ring.
While the above accomplishes a small-emittance electron beam, the ions and protons need to be cooled by coherent electron cooling to have small emittance. The eRHIC interaction region design relies on the existence of small emittance beams with a longitudinal RMS of 5 cm , resulting in $\beta^{*}=5 \mathrm{~cm}$. Strong focusing is obtained by three high-gradient quadrupole magnets using recent results from the LHC quadrupole magnet upgrade program (reaching gradients of $200 \mathrm{~T} / \mathrm{m}$ at 120 mm aperture). To ensure the previously described requirements from physics are met, four major requirements need to be fulfilled: high luminosity ( $>100$ times that of HERA), the ability to detect neutrons, measurement of the scattered proton from exclusive reactions (i.e. DVCS) and the detection of low-momentum
protons ( $\mathrm{p} \sim \mathrm{p}_{0} / 2.5$ ) from heavy-ion breakup. The eRHIC IR design fulfills all these requirements: the first magnet in the high focusing quadrupole triplet is a combined function magnet producing a 4 mrad bending angle of the ion/proton beam (see fig. 7.30). The 120 mm diameter aperture of the last quadrupole magnet allows detection of neutrons with a solid angle of $\pm 4 \mathrm{mrad}$, as well as the scattered proton from exclusive reactions, i.e. DVCS, up to a solid angle of $\sim 9 \mathrm{mrad}$. The electrons are transported to the interaction point through the heavy ion/proton triplets, seeing zero magnetic field as shown in fig. 7.30 .


Figure 7.30. Combined-function magnet of the hadron beam high focusing quadrupole triplet.
Fig. 7.31 shows the current eRHIC interaction region design in the direction of the outgoing hadron beam. The other side of the IR is mirror symmetric for the incoming hadron beam. For the outgoing lepton beam we are currently investigating how to best integrate a low scattering-angle lepton tagger. Such a tagger is critical for any low $Q^{2}$ physics, like elastic $J / \psi$ production in eA collisions (see section 5.14).


Figure 7.31. Schematic view of the eRHIC interaction region design in the direction of the outgoing hadron beam.

The scattered proton from DVCS events were tracked through this design and beam optics using HECTOR [1284. The DVCS events have been generated with MILOU, a MC
code dedicated to DVCS [673. From fig. 7.32 it is clear that protons from DVCS events can be measured in 'Roman Pots' after the high-focusing quadrupole triplet with a high detection efficiency for hadron beam energies starting from 100 GeV (as example are shown the results for 50 GeV and 250 GeV ). More studies are needed to determine the momentum and angular resolution that can be achieved depending on the 'Roman Pot' design.

As pointed out previously, equally challenging is the detection of the breakup neutrons from heavy ions to veto incoherent events. The nuclear breakup of Au nuclei depending on the excitation energy $\mathrm{E}^{*}$ was simulated using the Monte Carlo generator GEMINI++ [1285] and SMM [1286]. The MC simulation showed that whenever the nucleus breaks up there will be at least one neutron emitted. At very low excitation energies there is the possibility that only a photon is emitted, while the nucleus remains intact. The possibility of detecting these photons still needs to be investigated. Fig. 7.33 shows the angular distribution of the breakup neutrons for three different excitation energies. The aperture of 120 mm diameter of the last quadrupole magnet allows detection of neutrons with a solid angle of $\pm 4 \mathrm{mrad}$, which is indicated by the simulations to be sufficient.

Fig. 7.34 shows the detection inefficiency for these neutrons for three different excitation energies as function of the maximal aperture of the last magnet. For apertures discussed for the IR design the inefficiencies are $10^{-2}$ or much lower for all excitation energies. This assumes a $100 \%$-efficient zero degree calorimeter (ZDC). The critical question is: to suppress incoherent events at high $t$ in eA collisions, can the detection inefficiencies be controlled on the $10^{-3}$ to the $10^{-4}$ level?

There are many detector, interaction region and machine parameters still to be worked out in detail, but one of the hardest questions for an EIC will be to estimate the limiting factors for the systematic uncertainties. Due to the high luminosity, many inclusive and semi-inclusive physics observables will be systematics-limited after a relatively short time of data taking, assuming a $50 \%$ operations efficiency. This requires great care to be taken to consider the possible systematic limitations from the beginning and to integrate solutions to minimize them into the design. Only some of the possible limiting systematic effects that will need to be addressed with great care in the design are listed here. Their impact on key physics observables still needs to be studied.

- Absolute luminosity measurements between different beam energy combinations. This is extremely important for measurements like the structure function $\mathrm{F}_{L}$.
- Relative luminosity measurements between bunches with different bunch helicities, i.e. ,,++---+ and +- . Here it will be important to investigate whether Bremsstrahlung can be used for this measurement, as the Bremsstrahlung cross section has a term that is dependent on polarization.
- The measurements of the absolute hadron and electron beam polarization. To date the best precision in the measurement of lepton beam polarization at high energies in a collider was obtained during HERA-I running with $1.6 \%$ [1287. At RHIC the best hadron polarization measurement achieved to date is $\sim 5 \%$ [1288, 1289, 1290] for a polarized proton beam. For high energy polarized ${ }^{3} \mathrm{He}$ beams, $\mathrm{R} \& \mathrm{D}$ is needed to determine how to measure an absolute polarization.


Figure 7.32. Row-1: Spatial distribution of the scattered protons from DVCS events at 20 m from the IP for 2 different beam energy combinations. Row-2: As Row-1, applying the aperture limitations due to the magnets. Row-3: As Row-2, applying the limitations due to the $10 \sigma$ beam clearance and the acceptance of 'Roman Pots' as currently used by pp2pp at STAR. Row-4: Comparison of the $p_{T}$ spectrum of generated protons (black), those accepted by the quadrupole aperture (blue) and those detected in the 'Roman Pots' (red).


Figure 7.33. The angular distribution of neutrons from the breakup of a Au nucleus depending on the excitation energy.


Figure 7.34. The inefficiency to detect the neutrons from the breakup of a Au-nucleus as function of the maximal aperture of the last magnet for different excitation energies.

## ePHENIX

PHENIX is one of the two large dedicated RHIC detectors, located at IP-8. The PHENIX detector consists of two muon spectrometer arms and two central arms sitting in a 1 tesla solenoid. Over the years the detector has been upgraded to the configuration shown in fig. 7.35, Fig. 7.35 and the upper plot of fig. 7.36 show clearly that PHENIX


Figure 7.35. A schematic view of the current (2011) configuration of the PHENIX detector.
in its current configuration has only a very small acceptance $(|\eta|<0.35)$ for the scattered lepton. This makes the current PHENIX detector basically not usable for DIS physics.

For the RHIC decadal plan covering the period 2010-2020, PHENIX has proposed a major upgrade of the current detector [1291]. The decadal plan outlines an exciting program


Figure 7.36. Rapidity coverage of the current PHENIX detector compared to the strawman new PHENIX detector. The central barrel detector covers $|\eta|<1.0$; the forward detector has tracking coverage for $-4<\eta<-1$, with full EMCal and HCAL coverage for $-4.0<\eta<-2.0-(-1.5)$ with the exact range dependent on the final design configuration


Figure 7.37. Schematic drawing of the new PHENIX detector.
in heavy ion and spin physics in polarized pp collisions, focused on an investigation of the interplay between perturbative and nonperturbative physics in QCD and on the relative importance of strong and weak coupling. The physics aims have been translated into an extensive set of required physics observables to answer the key scientific questions, leading to the design of the new PHENIX detector. The upgrade plan involves replacing the PHENIX central magnet with a new compact solenoid. The limited aperture provided by the outer central arm detectors would be replaced with a compact EMCal and a Hadronic Calorimeter covering two units in pseudorapidity and full azimuth, complemented by the existing VTX and FVTX inner silicon tracking. Two additional tracking layers would be added. We highlight that the large acceptance and excellent detector capability is combined with high rate and bandwidth. The limited forward coverage of the current PHENIX detector does not allow one to adequately address the questions driving the nucleon structure and cold nuclear matter community, nor does it provide any capabilities for $\mathrm{e}+\mathrm{p}$ or $\mathrm{e}+\mathrm{A}$ collisions. Hence, an upgrade is being considered where one muon arm would be replaced by a new largeacceptance forward spectrometer with excellent PID for hadrons, electrons, and photons and full jet reconstruction capability. The modified detector layout is shown schematically in fig. 7.37. The increase in overall acceptance is shown in the lower part of fig. 7.36. The new compact barrel component at midrapidity is designed for excellent jet reconstruction and PID for photons, electrons, and $\pi^{0}$ in $\mathrm{p}+\mathrm{p}$, proton-nucleus, through central nucleusnucleus collisions. The forward upgrade design is driven by nucleon structure physics and cold nuclear matter physics. Such a forward spectrometer added to PHENIX would not only allow measurements of the single spin asymmetry at forward rapidity to test the QCD prediction that the Sivers function in Drell-Yan and SIDIS is opposite, but would also allow the unique possibility to detect the scattered lepton in $\mathrm{e}+\mathrm{p} / \mathrm{e}+\mathrm{A}$ collisions in the era of an eRHIC to virtualities $\mathrm{Q}^{2}>0.1 \mathrm{GeV}^{2}$. To realize these physics goals it is necessary to upgrade significantly the current PHENIX detector to a detector with high acceptance at forward rapidity $1<\eta<4.0$.

The strawman design for the central barrel has already been described. The forward detectors of the strawman design consist of a RICH, a preshower, an EMCal, an HCal, and additional tracking detectors to provide good momentum definition of the particles going forward. This combination of detectors is motivated by both Drell-Yan and e+p/e+A physics to emphasize the detection of electrons with high efficiency and purity.

It must be stressed again that the PHENIX detector upgrades as discussed above are driven by $\mathrm{p}+\mathrm{p}, \mathrm{p}+\mathrm{A}, \mathrm{A}+\mathrm{A}$ physics. But, comparing the requirements for the physics program at an EIC as described in section 7.3.1, it becomes clear that this detector upgrade also provides opportunities to carry out an $\mathrm{e}+\mathrm{p}$ and $\mathrm{e}+\mathrm{A}$ physics program, referred to as ePHENIX. The upgraded PHENIX is well suited for

- Inclusive e+p physics to measure polarized and unpolarized structure functions.
- Inclusive $\mathrm{e}+\mathrm{A}$ physics to measure unpolarized structure functions and derive nuclear parton distribution functions (nPDFs).
- e+p / e+A physics involving charm and bottom
- Elastic diffractive physics, i.e. elastic vector meson production and deeply virtual Compton scattering. These measurements require the addition of 'Roman pot' detectors.
nearly independent of the center-of-mass energy and lepton and hadron beam combination. Unfortunately due to the limited PID capabilities of the ePHENIX design, most of the SIDIS physics program for an EIC will not be possible.

There are still several open question on the detailed performance of the upgraded PHENIX detector in ep / eA collisions, which need to be studied in the next months. Some examples are given below. Of course, some of these concerns can easily be solved by addressing them by design changes.

- How can ePHENIX be integrated in the current IR design of eRHIC?
- What does the current material budget do to the momentum and angular resolution of the scattered lepton?
- Does the current compact solenoid provide enough bending power to achieve sufficient momentum resolution for the scattered lepton at low $\mathrm{Q}^{2}$ ?
- How can a luminosity measurement for ep/eA collisions be integrated in the design?
- Are the currently planned electromagnetic calorimeter designs suited in energy resolution to separate leptons from hadrons via $E / p$, and to get the required resolution for the DVCS photon?


## eSTAR

STAR is the other of the two large dedicated RHIC detectors, located at IP-6. Fig. 7.38 shows STAR in the configuration anticipated in 2014.

The unique strength of STAR (solenoidal tracker at RHIC) [1292] is its large, uniform acceptance capable of measuring and identifying a substantial fraction of the particles produced in heavy ion collisions. The heart of STAR is its main tracking device: a TPC, covering full azimuthal angle and $\pm 1.5$ units of pseudo-rapidity. $\mathrm{A} \mathrm{dE} / \mathrm{dx}$ resolution of $\sim$ $8 \%$ can be achieved by requiring the tracks of charged particles to have at least 20 out of a maximum of 45 hits in the TPC. Detailed descriptions of the TPC and its electronics system have been presented in [1293, 1294. The TPC sits in a 0.5 tesla solenoid, surrounded by electromagnetic calorimetry (EMC Barrel, EMC End Cap, FMS) covering $-1<\eta<4$, muon identification (MTD) covering $-1<\eta<1$ and a high-resolution time of flight system (MRPC ToF Barrel) covering $-1<\eta<1$. The tracking in STAR will be further improved by 2014 by adding a forward GEM tracker (FGT) covering $1<\eta<2$ and a high-resolution silicon detector (HFT) covering $-1<\eta<1$. The HFT gives the possibility to separate events with charmed mesons from those with beauty mesons through the detection of the displaced vertex for charmed mesons. Identification in the lepton sector will be enhanced with the Muon Telescope Detector (MTD), which will tag muons for $-1<\eta<1$. This will enable dilepton studies in the $\mu-\mu$ and $e-\mu$ channels, with a focus on separating the Upsilon states and constraining charm backgrounds to the thermal continuum in intermediate mass dileptons. Another unique feature of STAR is the 'Roman Pots' around the main detector; their main focus is to detect protons from elastic diffractive events in pp collisions.

In addition to large coverage in tracking and electromagnetic calorimetry, STAR has good particle identification capabilities. For stable charged hadrons, the TPC provides $\pi / \mathrm{K}(\pi+\mathrm{K} / \mathrm{p})$ identification to $\mathrm{p}_{T} \sim 0.7(1.1) \mathrm{GeV} / \mathrm{c}$ by the measurement of ionization energy loss ( $\mathrm{dE} / \mathrm{dx}$ ). The STAR PID capability is further enhanced by the TOF system with a time resolution of $<100 \mathrm{ps}$, which is able to identify $\pi / \mathrm{K}(\pi+\mathrm{K} / \mathrm{p})$ to $\mathrm{p}_{T} \sim 1.6$ (3.0)


Figure 7.38. Schematic drawing of the STAR detector in 2014.


Figure 7.39. Left: $1 / \beta$ vs. momentum for $\pi^{ \pm}, K^{ \pm}$, and $(p \bar{p})$ from $200 \mathrm{GeV} \mathrm{d}+\mathrm{Au}$ collisions. Separation between pions and kaons (kaons and protons) is achieved up to $\mathrm{p}_{T} \sim 1.6$ (3.0) $\mathrm{GeV} / \mathrm{c}$. The insert shows $m^{2}=p^{2}\left(1 / \beta^{2}-1\right)$ for $1.2<p_{T}<1.4 \mathrm{GeV} / \mathrm{c}$. Right: Distribution of $\log _{10}(d E / d x)$ as a function of $\log _{10}(p)$ for electrons, pions, kaons and (anti-)protons. The units of $d E / d x$ and momentum $(p)$ are $\mathrm{keV} / \mathrm{cm}$ and $\mathrm{GeV} / \mathrm{c}$, respectively. The color bands denote the $\pm 1 \sigma d E / d x$ resolution.
$\mathrm{GeV} / \mathrm{c}$, as demonstrated in the left panel of fig. 7.39, In addition, with the relativistic rise of $\mathrm{dE} / \mathrm{dx}$ from charged hadrons traversing the TPC at intermediate/high $\mathrm{p}_{T}(>3 \mathrm{GeV} / \mathrm{c})$ and diminished yields of electrons and kaons at this $\mathrm{p}_{T}$ range, pions and protons can be identified up to very high $\mathrm{p}_{T}(\sim 10 \mathrm{GeV} / \mathrm{c})$ in $\mathrm{p}+\mathrm{p}, \mathrm{p}+\mathrm{A}$ and $\mathrm{A}+\mathrm{A}$ collisions (see right panel fig. 7.39).

STAR has, like PHENIX, provided a decadal plan outlining the physics program for $\mathrm{pp}, \mathrm{dA}$ and AA collisions in the next 10 years [1295]. Contrary to PHENIX, the STAR upgrade plans are much more moderate and focus on forward rapidity $(2<|\eta|<4)$. On the side of the STAR detector at which the FMS is situated, the plan is to improve charged particle tracking by adding more tracking planes to the FGT to cover rapidities $2.5<\eta<4$. To improve lepton/hadron and $\gamma / \pi^{0}$ discrimination, as well as baryon/meson separation, a RICH detector and a preshower detector will be added in front of the FMS. The addition of a hadronic calorimeter behind the FMS will further improve the lepton/hadron separation, as well as give the possibility of measuring the energy due to neutral particles in jet reconstruction. The motivation for this upgrade is, like in the case of the PHENIX forward upgrade, transverse spin physics in pp collisions (Sivers asymmetry in Drell Yan) and the study of cold nuclear matter, i.e. parton saturation at small $x$.

The upgrade in rapidity $-4<|\eta|<-1$ is driven solely towards improving the detection capabilities of STAR for the scattered lepton in ep/eA collisions during the era of eRHIC. Currently, proposals include the addition of tracking and electromagnetic calorimetry as well as an additional ToF for PID. For tracking, it is proposed to combine high-resolution with electron identification by for example integrating a Cherenkov detector in the tracking detector.

Combining all these upgrades in fig. 7.40 shows that STAR will have very good acceptance for both the scattered lepton and for the hadrons produced by the current jet at the first stage of eRHIC, with 5 GeV electron beams colliding with proton beams with energies as high as 325 GeV . From these figures it is also obvious that the upgrade at negative rapidity is essential to provide good coverage for the scattered lepton below $\mathrm{Q}^{2}$ of $10 \mathrm{GeV}^{2}$.


Figure 7.40. Kinematic coverage of the STAR detector in the ( $\mathrm{x}, \mathrm{Q}^{2}$ ) plane. Left: electron. Right: struck quark. The electron beam energy is 5 GeV , and the nucleus beam energy is $100 \mathrm{GeV} / \mathrm{u}$. Lines of constant laboratory energy of the electron and the struck quark are shown.

The list of questions which need to be answered is very similar to that listed in the ePHENIX section, and many further detailed simulations must be performed to understand in detail the performance of STAR for ep/eA collisions. However from the first studies it is
clear that eSTAR will be able to make key measurements such as:

- Inclusive e+p physics to measure polarized and unpolarized structure functions.
- Inclusive $\mathrm{e}+\mathrm{A}$ physics to measure unpolarized structure functions and derive nuclear parton distribution functions (nPDFs).
- Elastic diffractive physics, i.e. elastic vector meson production and deeply virtual Compton scattering. Here the great advantage is that eSTAR already possesses 'Roman pot' detectors.
- The good particle ID capabilities also open the possibility of studying many of the semi-inclusive observables in ep/eA collisions, i.e. to do a flavour separation of the quark polarizations to understand both the helicity structure and the transverse spin structure (via Sivers and Collins functions) of the proton.


### 7.3.4 Detector Design for MEIC/ELIC

The Jefferson Lab design of an EIC is based on a novel figure-8 ring-ring design optimized for polarization preservation. The initial version of this EIC is termed the Medium-Energy EIC, or MEIC, which is upgradable to a higher-energy version termed Electron Ion Collider, or ELIC. The MEIC/ELIC will have minimal impact on continued operation of the Jefferson Lab (JLab) 12 GeV fixed-target program.

The ring-ring design of the MEIC/ELIC allows simultaneous operation at high luminosity of multiple detectors located at different interaction points (IPs). Due to the nature of the figure-8, four IPs are foreseen with different functions. The MEIC detector/interaction region has concentrated on maximizing acceptance for deep exclusive processes and processes associated with very-forward going particles, which are the most challenging from the detector point of view. This section will describe the baseline full-acceptance detector in more detail, where it is understood that the various MEIC/ELIC interaction points can house detectors employing different technologies and having a slightly different physics focus.

Given that the detailed design of various subsystems does not have to be frozen for another decade or so, and dedicated pre-R\&D projects are only now under way, the focus of the JLab effort has been on formulating requirements, identifying and addressing critical design issues, and integrating the detector with the interaction region of the accelerator. A tentative detector configuration with estimates based on realistic projections has been adopted, however, to provide users with input for simulations.

## The Medium-energy EIC (MEIC)

The current effort is geared towards the MEIC, for which the guiding principle has been based upon science motivation and design choices close to present state-of-the-art whenever possible. The exception to the latter is the ion beam properties, which have been established for electron-positron colliders but fundamentally depend on electron cooling for proton/ion beams. The fundamental choice for the MEIC design has been to assume short bunches, each carrying a small charge, and to achieve the requirements for the proton beam quality assume extrapolations from conventional electron cooling that have been successfully employed at Fermilab, albeit at modest proton energies. Extending this technology may be incremental, rather than transformational in nature.

While ELIC would have a circumference of about 3 km , and support proton energies up to 250 GeV (as well as heavy ions up to $100 \mathrm{GeV} / \mathrm{A}$ ), and electrons post-accelerated up to about 20 GeV , the MEIC would be somewhat smaller than the 1.4 km of the CEBAF accelerator, from which it would inject electron or positron beams between 3 and 11 GeV . The maximum proton energy would be around 100 GeV (or $40 \mathrm{GeV} / \mathrm{A}$ for heavy ions), but the often quoted design point for which performance parameters are being worked out in detail, is 60 GeV . The choice of a mid-range energy for these studies is primarily based on two considerations. On the accelerator side, a proton energy of 60 GeV is a somewhat more conservative value for which one could anticipate the performance projections for the electron cooling to become valid at an early stage of operations. On the physics side, a range of measurements, for instance related to the 3D structure of the nucleon, place strong demands on the resolution in $t$ and the luminosity at modest values of proton energy, corresponding to $s \sim 2000 \mathrm{GeV}^{2}$.

To further illustrate the importance of a mid-range energy for detailed imaging studies through exclusive reactions, we come back to the kinematics associated with these processes, but for a cut in $Q^{2}>10 \mathrm{GeV}^{2}$, a likely must for the valid partonic interpretation of such studies. If one implies a $Q^{2}>10 \mathrm{GeV}^{2}$ cutoff in such exclusive processes, the kinematic patterns of earlier fig. 7.20 drastically change. The upper panels of fig. 7.41 shows how the momentum distribution of mesons associated with exclusive pseudoscalar meson production change with lepton and proton energy. Compared to fig. 7.20, the peak in the forward-ion direction has disappeared completely. Lower lepton energies also push towards lower hadron momenta in the central-angle region, and thus reduced particle identification requirements. The bottom panels of fig. 7.41 show one of the most challenging constraints on the detector and interaction region design for exclusive reactions from the need for detection of the exclusive hadronic state remaining in the exclusive process. The figures show the direct correlation between $t$ and proton energy, scaling like $1 / E_{p}$, and shows the remaining baryonic state goes very much in the forward-ion direction, but far less so (and with lower momenta) for lower proton energies, which are thus much easier to peel off from any beam-stay-clear area. Even more, assuming a fixed resolution in $t$, there are obvious benefits of lower proton energies for imaging. Of course, any high-energy ELIC would in turn greatly benefit from the experience gained from the construction and operation of the MEIC.

While maintaining a future upgrade path to the high-energy ELIC is important and always folded into the MEIC design, emphasis has been placed on ensuring that ELIC will not simply supersede the MEIC, but rather provide a complementary capability. The MEIC is thus designed to excel in the kinematic range that it will cover (i.e., on one hand having an overlap with JLab 12 GeV , and on the other with HERA data with $y<0.3$ ). Overlap in science goals is in part achieved by various accelerator features. Perhaps one of the most prominent is the figure- 8 shape, which could allow storage of polarized deuterium beams. By tagging the spectator proton in the small-angle ion spectrometer (discussed below), this will allow to carry out measurements on quasi-free (polarized) neutrons. A high luminosity over a broad kinematic range will make it possible to accumulate sufficient statistics for multiple beam energy settings. The capability to vary the beam energies is essential for some measurements (e.g., $F_{L}$ ), but also makes it possible to optimize the data taking by reducing reliance on data taken at extreme values of $y$, where the systematic uncertainties grow. This can be achieved by having a lepton beam energy that can be varied continuously, and a series of closely spaced discrete ion beam energies. In the MEIC, the latter can be accomplished by changing the number of stored ion bunches by one, and the bunch separation distance accordingly - a scheme facilitated by the high bunch repetition


Figure 7.41. The momentum distribution of the exclusive hadronic final state as a function of the scattering angle for three different center of mass energies, $\sqrt{s}=31.6,44.7,100 \mathrm{GeV}$ (upper three panels), and the $t$ distribution as a function of scattering angle of the recoiling baryon in exclusive reactions for proton beam energies $E_{p}=50 \mathrm{GeV}$ and 250 GeV (lower two panels). A cut of $Q^{2}>10$ $\mathrm{GeV}^{2}$ is applied to select the kinematic range of interest for exclusive processes. For lower center of mass energies, the momentum distribution tends towards more central scattering angles and covers lower momenta. The angle of the recoiling hadronic system is directly and inversely correlated with the proton energy. It thus decreases with increasing proton energy. For instance, as shown here, the baryon scattering angle ranges to about $1-2^{\circ}$ at a proton energy of 50 GeV and is reduced to one fifth of that as the proton energy increases to 250 GeV .
frequency. Independently varying beam energies also makes it possible to choose the most suitable lab kinematics at a certain value of $s$, potentially improving acceptance, resolution, and particle identification for the reaction of interest (see also fig. 7.41).

Having small, short ion bunches with a high bunch repetition frequency also facilitates the use of SRF crab crossing cavities, which were originally developed for KEKB to allow beams collide at an angle without significant loss of luminosity. In the context of an EIC, these were pioneered in the ELIC design, and the possibility of creating a significant crossing angle (at least 50 mrad ) became early on a key feature of the small-angle detection for the MEIC (see section 7.3.4).

## Detector Placement and Backgrounds

The figure-8 ring can support two IPs per straight section, one of which will be a "highluminosity" IP with the full crossing angle. In order to minimize backgrounds, the two high-luminosity IPs will be located close to where the ion beam exits the arc, and far away from the arc where the lepton beam exits. The latter helps to decrease synchrotron radiation (and the secondary neutron flux) at the IP, which is anyway already reduced due to the use of crab crossing (with the ion beam, not the electron beam, making the horizontal bend correction). The synchrotron background is reduced even further by lowering the strength of the last arc dipoles. The short distance between the ion arc and IP suppresses detector backgrounds from interactions of the beam with residual gas in the beam pipe by providing a smaller "target" with line-of-sight to the detector. A shorter section of the beamline is also easier to bake and keep at at ultra-high vacuum. A comparison with HERA, also taking into account the lower $p-p$ (and $p-A$ ) cross section and lower hadron multiplicity at the 100 GeV , suggests that the hadronic background will be about an order of magnitude lower in the MEIC at comparable vacuum and ion beam current, leaving a lot of headroom to increase the latter. Due to the bends associated with the horizontal crossing, the secondary IPs on each straight section will not have a line-of-sight along the full straight section, but there this is less of an issue since they are intended to either have diagnostics equipment (e.g., polarimetry), or special detectors which are less sensitive to backgrounds or intended to operate at lower beam currents.

## Detector and Interaction Region Layout

A global outline of the fully integrated MEIC detector and interaction region is given in fig. 7.42, We will in the subsequent subsections go in more detail over the central detector region, defined as the region of the detectors operating within the solenoid, the electron and ion endcaps, and the strategy to accomplish a full-acceptance detector. The latter has two ingredients, a relatively simple approach to incorporate low- $Q^{2}$ electron detection and a more challenging solution to measure forward and ultra-forward (in the ion direction) going hadronic or nuclear fragments. Here, we make critical use of various ingredients of the MEIC detector/interaction region design: i) the 50 mrad crossing angle; ii) the range of proton energies; iii) a small 1-2 Tm dipole field to allow measurement down to $0.5^{\circ}$ before the ion final focusing magnets; iv) ion final focusing magnets with apertures sufficient for particles with angles up to at least $0.5^{\circ}$; and v) a large 20 Tm dipole field much more downstream to peel off spectator particle and allow for very small-angle detection.

The strategy will be that various detector elements, amongst which zero degree calorimeters for neutron detection and various small-angle detectors, will be placed in the region


Figure 7.42. Interaction region and central detector layout, and its placement in the general integrated detector and interaction region. The central detector includes endcaps in both the electron and ion direction.
between the ion final focusing quads and the 20 Tm dipole field, and also beyond this 20 Tm dipole field. This then results in an essentially $100 \%$ full acceptance detector. The electron beam traverses the center region of the solenoid, while the proton/ion beam traverses at the crab crossing angle. This choice minimizes any electron steering and synchrotron radiation. Note that the 50 mr crab crossing angle also facilitates the small-diameter electron final focusing quads to be moved in to 3.5 meter distance of the interaction point. The lower electron beam energies and hence lower-field requirements for the electron beam allows the construction of relatively small-sized quadrupoles, much simplifying the electron optics design.

## Central Detector

To fulfill the requirement of hermeticity, the central detector will be built around a solenoid magnet (with a length of about 5 m ). Due to the asymmetric beam energies, the interaction point (IP) will be slightly offset towards the electron side $(2 \mathrm{~m}+3 \mathrm{~m})$. This will allow more distance for the tracking of high-momentum hadrons produced at small angles, and a larger bore angle for efficient detection of the scattered beam leptons.

The characteristics of the solenoid are guided by the desire to optimize the tracking resolution, which at central angles scales like $\Delta p / p \sim \sigma p / B R^{2}$, where $\sigma$ is the position resolution, $p$ the particle momentum, $B$ the magnetic field, and $R$ the radius of the central tracker. At forward angles, however, the resolution depends on the scattering angle, but is independent of $R$ as the particle leaves the cylindrical central tracking system from the front side (see the left panel of fig. (7.43). The resolution will then deteriorate rapidly given the lack of transverse field along the central axis of a solenoid. This will later be remedied
by adding a small dipole field, as high ion energies boost the outgoing hadrons to high momenta at forward angles and one wishes to optimize resolutions also in the forward-ion direction. To obtain a roughly better than $1 \%$ momentum resolution for central angles and particles in the $5-10 \mathrm{GeV} / \mathrm{c}$ momentum range, a field $B$ in the 2-4 T range seems highly desirable. This high field requirement suggests a magnet with a reasonably small diameter, preferably not larger than about 4 m , putting radial space at a premium. Of course, a smaller diameter has the advantage of simplifying the magnet design, with the additional advantage of reducing detector cost (which scale with the radius for the barrel calorimeter and roughly as the radius squared for the endcaps). An alternate solution may be to increase the space for tracking in the central solenoid while reducing the required solenoid field, as illustrated in the right panel of fig. 7.43, Here, the resolution improvement for pions with $10 \mathrm{GeV} / \mathrm{c}$ momentum and a scattering angle of $90^{\circ}$ is shown as a function of the tracking length and solenoidal field. Thus, there is strong incentive to reduce the space requirements for particle identification detectors within the central solenoid as much as possible, to use available space for tracking, or reduce the solenoid diameter.


Figure 7.43. (left) The resolution as a function of lab angle for a particle (pion) momentum of 5 $\mathrm{GeV} / \mathrm{c}$ in a 4 T ideal solenoidal field and with a cylindrical tracker of radius 1.25 m ; (right) The resolution as function of solenoidal field strength and tracker radius for a particle (pion) momentum of $10 \mathrm{GeV} / \mathrm{c}$ and a scattering angle of $90^{\circ}$.

The central detector would contain a tracker, particle identification, and calorimetry. A three layer configuration of the central tracker was suggested at the JLab EIC detector workshop (June 4-5, 2010)2. The first layer would consist of a low-mass vertex tracker with sufficient resolution to separate primary and secondary vertices in charm production. The middle layer would be a Time-Projection Chamber (TPC) with GEM-based readout, and the outer layer would be a cylindrical GEM tracker. The position resolution of the TPC would be about $50 \mu \mathrm{~m}$, which is a factor two improvement over the inner drift chambers of CLAS12. In conjunction with the outer GEM layer, it should provide adequate $(r, \theta, \phi)$ in-

[^289]formation. Ongoing R\&D for vertex and micropattern detectors (including GEMs), suggest that such a high-performance tracker could be built for the EIC detector. Nevertheless, a radius of at least 1 m would be required.

Particle identification in the central detector is the most open design question. At low momenta, $\mathrm{dE} / \mathrm{dx}$ (in the TPC) or TOF can be helpful. With precise timing, the momentum range of the latter could be extended somewhat (although this would require a comparable uncertainty on the track length determination in order to get a good $t_{0}$ ). The most challenging requirement is, however, for a radially compact detector providing $\pi / K$ identification over a sufficiently wide momentum range. Taking up 8 cm of radial space, a BaBar-type DIRC could satisfy this condition, providing $3 \sigma \pi / K$ separation up to $4 \mathrm{GeV} / \mathrm{c}$, e/ $\pi$ separation close to $1 \mathrm{GeV} / \mathrm{c}$, and p/K separation up to $7 \mathrm{GeV} / \mathrm{c}$. An aerogel barrel RICH could provide almost comparable performance. Neither is sufficient for the exclusive (GPD) or semi-inclusive (TMD) programs. The current baseline design thus includes a Low-Threshold Cherenkov Counter (LTCC) with $C_{4} F_{10}$ or $C_{4} F_{8} O$ gas in addition to the DIRC. This would provide $e / \pi$ separation between 1 and $3 \mathrm{GeV} / \mathrm{c}$, and $\pi / K$ separation from 4 to $9 \mathrm{GeV} / \mathrm{c}$, but at a price of $50-70 \mathrm{~cm}$ of radial space. Adding $C_{4} F_{10}$ to a barrel RICH would increase the radius by at least $80-90 \mathrm{~cm}$, although a RICH could extend the momentum coverage to $14 \mathrm{GeV} / \mathrm{c}$. Ultimately the allocation of radial space to PID and tracking is a matter of priorities, and with multiple detectors one could easily imagine that these would offer complementary capabilities. On the other hand, if one could improve the $\theta_{c}$ resolution for a DIRC by about a factor of two, its $3 \sigma \pi / K$ separation could be extended to about $6 \mathrm{GeV} / \mathrm{c}$, with the upper limits for the other particle species shifting accordingly, eliminating the need for the gas Cherenkov. Given the size of the EIC detector, an all-crystal electromagnetic calorimeter would be financially expensive and only needed in critical regions. Tungsten powder / scintillating fiber or other technologies may provide a more affordable alternative for the barrel without an excessive loss of resolution. If needed, the return yoke of the solenoid magnet can be used as part of a hadronic calorimeter, and as an absorber for muon detection (along the lines of CMS).

## Detector Endcaps

The electron side endcap would face requirements quite similar to those of CLAS12, and it is natural to adopt a similar design. Due to the offset of the IP, lower particle momenta, and simpler small-angle detection (see section 7.3.4), the electron side is not nearly as crowded as the ion one. For lepton detection at small polar angles ( $\theta$ ), the main priority of the tracking would be to provide good $\theta$ resolution, as this directly impacts the reconstruction of the event kinematics. The inner part of the endcap tracker should thus be an extension of the vertex tracker, using semiconductor detectors. At larger angles, the requirements are not as demanding and the choice of technology is not as crucial. It could include planar GEMs or even cheaper drift chambers with a small cell size. Given the generous space constraints, a final tracking region could be added outside of the solenoid itself to improve tracking performance. Lepton identification will also use an electromagnetic calorimeter and a High-Threshold Cherenkov Counter (HTCC) with $C F_{4}$ gas or equivalent. The light can be collected by mirrors, producing a cost-effective readout. In this endcap region, hadron identification will be partially provided by a TOF detector, for which the endcap is more suitable than the barrel due to the longer flight path. The $\pi / K$ identification range, again in the electron endcap region, could be extended through the use of a LowTheshold Cherenkov Counter (LTCC) with $C_{4} F_{8} O$ gas or equivalent, possibly operating
slightly above atmospheric pressure to lower the pion detection threshold. Of course, to push $\pi / K$ identification to larger momenta, $\sim 10 \mathrm{GeV} / \mathrm{c}$, a RICH detector may need to be considered, but there does not seem to be a compelling need in this electron endcap region for the MEIC. Given the space available on the electron side, there is no strong requirement for a compact electromagnetic calorimeter. Since the momentum resolution from tracking deteriorates at small angles, where also the rates go up, the ideal configuration would involve an inner circle of high-resolution, radiation-hard crystals, and a more budget-friendly outer part. Both could be covered by the same pre-shower calorimeter.

The ion side endcap would have to deal with hadrons with a wide range of momenta, some approaching that of the ion beam. The forward tracking would thus greatly benefit from good position resolution (e.g., planar GEMs), at least on par with the $50 \mu \mathrm{~m}$ of the TPC. The smallest angles can be covered by semiconductor detectors as on the electron side. Of course, a good position resolution will also put significant demands on the detector alignment and field knowledge. The most important feature of the forward tracker, however, is related to the ion beam crossing angle with respect to the electron beam. In addition to being a key component of the small-angle detection, this turns the tracking resolution into a 2D problem. Whereas the momentum resolution in a solenoidal field deteriorates rapidly at small angles with respect to the axis, the hadron scattering angle is essentially defined with respect to the ion beam line. Given that the proton/ion beam traverses the solenoid at a 50 mr (crab crossing) angle, so already encounters some transverse magnetic field component, hadrons scattered away from the electron beam will end up in a part of the detector with better momentum resolution than those scattered towards the electron beam. Taking the 2D character of the problem into account, and the significant 50 mr beam crossing angle, the spot of poor resolution will be moved into the periphery covering and only a small range in the azimuthal angle $\phi$ will be affected. For most processes, all particle tracks will remain in the zone of good resolution. In contrast, if the crossing angle is small, all particle tracks at very forward angles will suffer from poor momentum resolution, as shown in the right panel of fig. 7.43 ,

To identify particles of various species over the full momentum range, one would ideally want to use several radiators. A typical combination could include aerogel (perhaps with more than one index of refraction), $C_{4} F_{10}$ or equivalent gas, and $C F_{4}$. This would make some kind of RICH detector an attractive option, in particular if the endcap radius was not too large. Still, there are several possible approaches which eventually will need to be studied in detail. One could, for instance, imagine a dual radiator gas RICH combined with a disk DIRC (as in PANDA), with the latter providing $\pi / K$ identification up to about $4 \mathrm{GeV} / \mathrm{c}$. Having the longest flight path from the IP, the ion endcap is also where one could achieve the best results with high-resolution TOF (perhaps even integrated with the readout of the RICH). Regardless of technical solution, the total thickness of the stack of PID detectors is assumed not to exceed 1.5 m . Calorimetry in the ion endcap will include both electromagnetic and hadronic parts. The main focus of the former will be to study various reaction products rather than the scattered lepton. However, the same resolution arguments apply as for the electron endcap, and a solution with an inner high-resolution circle, and a more cost-effective outer part makes sense here as well. The magnetic enclosure of the endcap can, as in the case of the return yoke of the central detector, be integrated with a hadronic calorimeter, and serve as an absorber for muon detection.

## Small-angle Detection

The design for the full-acceptance detector envisions small-angle detection on both sides of the central detector. The naming convention used here will be that the "ion side" or "ion endcap" refers to the side of the outgoing ion and incoming electron beam. The "electron side" refers to the other one.


Figure 7.44. Forward ion detection with 50 mrad crossing angle for the full-acceptance detector. Note that the distance to the final focusing quadrupoles are located 7 m from the IP.

On the ion side, the detection will be performed in three stages as illustrated in fig. 7.44. The first stage is the endcap (discussed in section 7.3.4), which will cover all angles down to the acceptance of the forward spectrometer. This in turn has two stages, one upstream of the ion Final Focus Quadrupoles (FFQs), covering down to $0.5^{\circ}$, and one downstream covering up to at least $0.5^{\circ}$. The former will use a 1-2 Tm dipole to augment the solenoid in the range where the resolution is poor. The magnet will be about 1 m long and cover the distance to the electron beam (corresponding to the horizontal crossing angle of 50 mrad ), and about twice that in the other directions, for a total acceptance of 150 mrad in the horizontal and 200 mrad in the vertical plane. An important feature of the magnet design is to ensure that the electron beam line stays field free. The dipole will have trackers at the entrance and exit, and a calorimeter covering the ring-shaped area in front of the first ion FFQ. For neutrons, the primary goal of this calorimeter is to have good angular resolution. This intermediate stage is essential for providing good coverage and resolution in $-t$, and to investigate target fragmentation. The former is of particular importance for the study of exclusive processes, essential for the 3D imaging of the nucleon, requiring detection of the recoil baryon. Since $t \sim \theta_{p}^{2} E_{p}^{2}$, the $t$-resolution depends on the angular resolution that can be achieved. With a 50 GeV proton beam, a $-t$ of $1 \mathrm{GeV}^{2}$ corresponds to about 27 mrad (see fig. (7.41). With an angular resolution of 1 mrad , the intermediate detection stage would be able to cover $-t$ up to $2 \mathrm{GeV}^{2}$ with a resolution of about $40-50 \mathrm{MeV}^{2}$ a value that would scale with angular resolution of the inner silicon forward tracker. Recoil baryons with larger values of $-t$ would be detected in the endcap. At higher ion beam energies the $t$-acceptance of the dipole increases, but the resolution deteriorates rapidly (due to the $E_{p}^{2}$ factor). Going to lower ion energies, the opposite is true.

The last stage is the ultra-forward detection that is crucial for the tagging of spectator protons in deuterium, as well as other recoil baryons/nuclei. The design is heavily integrated with the accelerator (see fig. 7.45), using two key features. One is, again, the horizontal crossing angle for the ion beam, which needs to be "corrected" some distance downstream of the interaction point (IP). For a 50 mrad crossing angle, this corresponds to a bend of close to 100 mrad , and the required 20 Tm dipole(s) can also serve as a dedicated forward spectrometer, using the long drift space beyond for detection of both charged and neutral


Figure 7.45. The integration of particle detection in the accelerator.
particles. The other feature is a beam optics requiring low quadrupole gradients, allowing large aperture magnets. In the current design, the maximum quad gradient is less than 65 $\mathrm{T} / \mathrm{m}$. With a 10 cm aperture, this creates a 6.5 T peak field (simply the product of the aperture radius and gradient), which the magnet design should be able to support if larger peak fields were acceptable, the apertures would increase accordingly. The gradients are further arranged so that they drop off faster than the distance from the IP to that specific location, allowing the apertures to become correspondingly larger, and thereby making sure that no bottlenecks are created. This defines a geometrical acceptance through the ion final-focusing quads (FFQs) of 10 mrad , or well beyond $0.5^{\circ}$, on each side of the beam ( 20 mrad in total). To focus the 250 GeV beams in ELIC, the maximum quadrupole gradients would have to be 2.5 times larger than for the 100 GeV of the MEIC, and the apertures reduced accordingly.

The acceptance for charged particles depends on both the polar and azimuthal angles (since quads focus in one plane and defocus in the other), as well as their momentum. This can be optimized by placing a dipole spectrometer relatively close to the FFQs. To give a numerical example, a 100 mrad bend to a deuterium beam would equate to a 200 mrad bend for a spectator proton. Over a drift space of 10 m (a relatively modest distance), the spectator proton would acquire a transverse separation of 1 m from the main beam. For heavy nuclei $(\mathrm{A} / \mathrm{Z}=2.5)$ with a negligible scattering angle at close to the beam momentum, this would increase to 1.5 m , while fragments with other $\mathrm{A} / \mathrm{Z}$ ratios would be lined up in between (in particular, $\mathrm{N}=\mathrm{Z}$ would be at 25 cm , while neutron rich fragments would be deflected to the other side). Ions scattered at zero degrees and having $98 \%$ of the beam momentum would be 2 cm from the beam after 10 m of drift. Due to the large deflection
in a well known field (including the few preceding elements), the momentum resolution of the spectrometer would be excellent. Since no position measurements would be possible within the beam-stay-clear area, the angular resolution would depend on the knowledge of the optics between the IP and detection point. The reconstruction of the angle would be aided by the scattered particles quickly exiting the beam-stay-clear area after having passed the spectrometer, with multi-point tracking to be applied in the drift region. Nevertheless, some some low-momentum particles scattered at large angles will not make it all the way to the dipole spectrometer. To detect these particles, some ad hoc detectors ("Roman pots") may be placed along the way, although an interesting idea currently under investigation is to have a small-diameter compensating solenoid between the FFQs and the 20 Tm dipole. In addition to its benefits for the accelerator, such a magnet could help in tracking charged particles that do not reach the final spectrometer dipole.

The low- $Q^{2}$ tagger on the electron side will complement the electron detection in the central detector and electron side endcap. Since the electron quad gradients required for 11 GeV beams are very small compared with what is needed for 100 GeV protons, one can make the apertures very large without being constrained by peak fields (the different apertures on the incoming and outgoing sides do not affect the optics). The optimal transition point from the calorimeter to tagger coverage will ultimately be determined by physics simulations. The quads would be followed by a dipole spectrometer with sufficient drift space ( 8 m in the current layout) to detect leptons with a significant fraction of the beam energy.

## Beam Helicity Reversals

The electron and ion beam polarimetry has been given a special "interaction region" in the MEIC/ELIC design, in part due to the often large amount of space needed for Compton polarimetry. With the anticipated work in systematic understanding of Compton polarimetry in both JLab Halls A and C, and further plans to cross-calibrate this with atomic beam Moller polarimetry for a future demanding parity-violating Moller experiment, electron beam polarization determination through Compton polarimetry may well achieve sub- $0.5 \%$ uncertainties. Ion beam polarimetry remains more complicated, although efforts to reduce uncertainties are underway and possibilities are studied in elastic and inelastic electron-proton scattering experiments in situ.

The MEIC design will need both fast electron spin helicity reversal or flip for double-spin experiments and a program of deep-inelastic parity-violating experiments, and fast ion-spin flip for single-nucleon spin asymmetry experiments. The latter can also be an alternate method for double-spin experiments. The MEIC design, with its 750 MHz bunch trains, does not assume bunch-to-bunch spin flips, but also does not need it. A helicity-reversal frequency of 0.1 Hz will be at about the level needed for experiments.

For double-spin experiments, it is to first order equivalent to perform fast helicity reversals of electron or ions. The choice is a question of detailed precision, as shown later. For single-spin asymmetry experiments, these techniques are however totally different, and can not replace each other. Single-electron spin asymmetry (flipping electrons only) is mostly useful for parity violation experiments, while single-nucleon spin asymmetry (flipping ions) is mostly useful for nucleon transverse-spin and other TMD experiments. Both type of experiments are routinely performed at JLab, and both will become an important part of the EIC science program.

The rate of the required helicity flips is closely related to the systematic understanding of the precision. Typically, although already very difficult, one can control the systematic
uncertainties between two helicity states to about $1 \%$. To further reduce this asymmetry, to a level of $10^{-8}$ for the case of typical parity-violating experiments at JLab, or to a level of $10^{-5}$ for transverse-spin experiments, one has to provide a suppression faction of $10^{-6}$ (for electron spin flip) or $10^{-3}$ (for ion spin flip) by fast spin flip techniques. The suppression factor by such fast helicity reversal is proportional to $1 / \sqrt{N}$, where $N$ is the number of pairs of spin flip. If we assume a typical single-nucleon spin asymmetry experiment of 3 months of continuous running (assuming one can keep control of the systematic uncertainties between the two helicity states at the $1 \%$ level for the full period), one needs to accumulate $10^{6}$ pairs to reach a suppression of 1000 , or about 8 flips per minute. This is the root of the present 0.1 Hz beam helicity reversal assumption mentioned above.

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# Terascale Physics Opportunities at a High Statistics, High Energy Neutrino Scattering Experiment: NuSOnG 

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#### Abstract

This article presents the physics case for a new high-energy, ultra-high statistics neutrino scattering experiment, NuSOnG (Neutrino Scattering on Glass). This experiment uses a Tevatron-based neutrino beam to obtain over an order of magnitude higher statistics than presently available for the purely weak processes $\nu_{\mu}+e^{-} \rightarrow \nu_{\mu}+e^{-}$and $\nu_{\mu}+e^{-} \rightarrow \nu_{e}+\mu^{-}$. A sample of Deep Inelastic Scattering events which is over two orders of magnitude larger than past samples will also be obtained. As a result, NuSOnG will be unique among present and planned experiments for its ability to probe neutrino couplings to Beyond the Standard Model physics. Many Beyond Standard Model theories physics predict a rich hierarchy of TeV -scale new states that can correct neutrino cross-sections, through modifications of $Z \nu \nu$ couplings, tree-level exchanges of new particles such as $Z^{\prime}$ s, or through loop-level oblique corrections to gauge boson propagators. These corrections are generic in theories of extra dimensions, extended gauge symmetries, supersymmetry, and more. The sensitivity of NuSOnG to this new physics extends beyond 5 TeV mass scales. This article reviews these physics opportunities.


## I. INTRODUCTION

Exploring for new physics at the "Terascale" - energy scales of $\sim 1 \mathrm{TeV}$ and beyond - is the highest priority for particle physics. A new, high energy, high statistics neutrino scattering experiment running at the Tevatron at Fermi National Accelerator Laboratory can look beyond the Standard Model at Terascale energies by making precision electroweak measurements, direct searches for novel phenomena, and precision QCD studies. In this article we limit the discussion to precision electroweak measurements; QCD studies and their impact on the precision measurements are explored in ref. [1, 2]. The ideas developed in this article were proposed within the context of an expression of interest for a new neutrino ex-
periment, NuSOnG (Neutrino Scattering On Glass) [1].
A unique and important measurement of the NuSOnG physics program is the ratio of neutral current (NC) and charged current (CC) neutrino-electron scattering, which probes new physics. The leading order Feynman diagrams for these processes are shown in Fig. 1. The NC process, $\nu_{\mu}+e^{-} \rightarrow \nu_{\mu}+e^{-}$, called "elastic scattering" or ES, provides the sensitivity to the Terascale physics. This process can explore new physics signatures in the neutrino sector which are not open to other, presently planned experiments. The CC process, called "inverse muon decay" or IMD, $\nu_{\mu}+e^{-} \rightarrow \nu_{e}+\mu^{-}$, is well understood in the Standard Model due to precision measurement of muon decay [3]. Since the data samples are collected with the same beam, target and detector at


FIG. 1: Left: "elastic scattering" (ES). Right:"Inverse Muon Decay" (IMD).
the same time, the ratio of ES to IMD events cancels many systematic errors while maintaining a strong sensitivity to the physics of interest. Our measurement goal of the ES to IMD ratio is a $0.7 \%$ error, adding systematic and statistical errors in quadrature. The high sensitivity which we propose arises from the combined high energy and high intensity of the NuSOnG design, leading to event samples more than an order of magnitude higher than past experiments.

Normalizing the ES to the IMD events represents an important step forward from past ES measurements, which have normalized neutrino-mode ES measurements to the antineutrino mode, $\bar{\nu}_{\mu}+e^{-} \rightarrow \bar{\nu}_{\mu}+e^{-}$[4, 5]. The improvement is in both the experimental and the theoretical aspects of the measurement. First, the flux contributing to IMD and $\nu \mathrm{ES}$ is identical, whereas neutrino and antineutrino fluxes are never identical and so require corrections. Second, the ratio of $\nu \mathrm{ES}$ to $\bar{\nu} \mathrm{ES}$ cancels sensitivity to Beyond Standard Model (BSM) physics effects from the NC to CC coupling ratio, $\rho$, which are among the primary physics goals of the NuSOnG measurement. In contrast, there is no such cancellation in the ES to IMD ratio.

The design of this experiment, described in Sec. II, is driven both by requiring sufficient statistics to make precision neutrino-electron scattering measurements and by the need for a neutrino flux which does not extend below the IMD threshold. The threshold for IMD events is

$$
\begin{equation*}
E_{\nu} \geq E_{\mu} \geq \frac{m_{\mu}^{2}}{2 m_{e}}=10.9 \mathrm{GeV} \tag{1}
\end{equation*}
$$

where we have dropped the small $m_{e}^{2}$ term for simplicity. The functional form above threshold, shown in Fig. 2, is given by $\left(1-m_{\mu}^{2} / E_{c m}^{2}\right)^{2}$, where $E_{c m}$ is the center of mass energy. Thus a high energy neutrino beam is required to obtain a high statistics sample of these events. The flux design should provide a lower limit on the beam energy of about 30 GeV , still well above the IMD threshold.

Sec. III describes the Standard Model Physics of neutrino electroweak scattering, for both electron and quark targets. In this section, the value of the normalization of the ES to IMD events is further explored. The very high statistics will also permit an electroweak measurement using the deep inelastic scattering (DIS) data sample from NuSOnG, via the "Paschos Wolfenstein method"


FIG. 2: Threshold factor for the IMD cross section, as a function of neutrino energy.
(PW) 6. The best electroweak measurement using DIS events to date comes from the NuTeV experiment, which has observed an anomaly. The status of this result is reviewed below. Making conservative assumptions concerning systematic improvements over NuTeV , our measurement goal using this technique is a $0.4 \%$ error on $\sin ^{2} \theta_{W}$, adding statistical and systematic errors in quadrature.

In Sec. IV, we discuss NuSOnG's potential to discover or constrain new physics through indirect probes, by making precision measurements of SM processes to look for deviations from SM predictions. We first frame the issue by considering in turn several model-independent parameterizations of possible new physics and asking what constraints will be imposed on new physics in the event NuSOnG agrees with the SM. (1) Oblique correction parameters describe the effects of heavy new states in vector boson loops. (2) New states may induce higherdimensional effective operators involving neutrinos. Finally, (3) new states may modify the couplings of the gauge bosons to neutrinos and leptons, including possibly violating lepton universality. In each case we consider the ability of NuSOnG to detect or constrain these types of deviations from the SM.

In Sec. V. we examine specific models for new physics. We begin by presenting the sensitivity to a set of new physics models. In particular, we consider

- typical $Z^{\prime}$ models,
- non-degenerate leptoquark models,
- R-parity violating SUSY models,
- extended Higgs models.

The models were selected because they are often used as benchmarks in the literature. While this list is not exhaustive, it serves to illustrate the possibilities. For each case, we consider how NuSOnG compares to other measurements and note the unique contributions. We end this section by approaching the question from the opposite view, asking: how could the results from NuSOnG clarify the underlying physics model, should evidence of new physics emerge from LHC in the near future?


FIG. 3: The assumed energy-weighted flux, from the NuTeV Experiment [7, in neutrino mode (left) and antineutrino mode (right). Black: muon neutrino, red: muon antineutrino, blue: electron neutrino and antineutrino flux.

Two further studies which can be performed by NuSOnG are QCD measurements and direct searches. The very large ( $\sim 600$ million event) DIS sample will allow the opportunity for precision studies of QCD. There are many interesting measurements which can be made in their own right and which are important to NuSOnG's Terascale physics program. The very high flux will also permits direct searches for new physics. Those which complement the physics discussed in this paper include:

- non-unitarity in the light neutrino mixing matrix;
- wrong-sign inverse muon decay (WSIMD), $\bar{\nu}_{\mu}+$ $e^{-} \rightarrow \mu^{-}+\bar{\nu}_{e} ;$
- decays of neutrissimos, i.e., moderately-heavy neutral-heavy-leptons, with masses above 45 GeV .

For more information on these studies, see refs. [1, 2,

## II. CONCEPTUAL DESIGN FOR THE EXPERIMENT

In order to discuss the physics case for a new high energy, high statistics experiment, one must specify certain design parameters for the beam and detector. The beam and detector should marry the best aspects of NuTeV [7], the highest energy neutrino experiment, and Charm II [9, the experiment with the largest ES sample to date. The plan presented here is not optimized, but provides a basis for discussion. The final design of the NuSOnG detector will be based on these concepts, and is still under development.

In this section, we present, but do not justify, the design choices. Later in this article, we discuss the reasoning for the choices, particularly in Secs. IIIC and IIID.

We will assume a beam design based on the one used by the NuTeV experiment [7], which is the most recent high energy neutrino experiment. This experiment used 800 GeV protons on target. The beam flux, shown in Fig. 3. is ideal for the physics case for several reasons. There is essentially no flux below 30 GeV , hence all neutrinos
are well above the IMD threshold. It is sign-selected: in neutrino mode, $98.2 \%$ of neutrino interactions were due to $\pi^{+}$and $K^{+}$secondaries, while in antineutrino mode $97.3 \%$ came from $\pi^{-}$and $K^{-}$. The "wrong sign" content was very low, with a $0.03 \%$ antineutrino contamination in neutrino mode and $0.4 \%$ neutrino contamination in antineutrino mode. The electron-flavor content was $1.8 \%$ in neutrino mode and $2.3 \%$ in antineutrino mode. The major source of these neutrinos is $K_{e 3}^{ \pm}$decay, representing $1.7 \%$ of the total flux in neutrino mode, and $1.6 \%$ in antineutrino mode.

Redesign of the beamline for NuSOnG is expected to lead to modest changes in these ratios. For example, if the decay pipe length is 1.5 km rather than 440 m , as in NuTeV , the $\pi / K$ ratio increases by $20 \%$ and the fractional $\nu_{e}$ content is reduced.

With respect to Tevatron running conditions, we will assume that twenty times more protons on target (POT) per year can be produced for NuSOnG compared to NuTeV . This is achieved through three times higher intensity per pulse (or "ping"). Nearly an order of magnitude more pulses per spill are provided. Our studies assume $4 \times 10^{19} \mathrm{POT} /$ year, with 5 years of running. Preliminary studies supporting these goals are provided in ref. 8].

The event rates quoted below are consistent with $1.5 \times 10^{20}$ protons on target in neutrino running and $0.5 \times 10^{20}$ protons on target in antineutrino running. The choice to emphasize neutrino running is driven by obtaining high statistics ES, which has a higher cross section for neutrino scatters, and to use the IMD for normalization this process only occurs in neutrino scattering. The Standard Model forbids an IMD signal in antineutrino mode. However, some antineutrino running is required for the physics described in the following sections, especially the PW electroweak measurement.

The beam from such a design is highly forward directed. NuTeV was designed so that $90 \%$ of the neutrinos from pion decay were contained within the detector face, where the detector was located at 1 km . For NuSOnG, which will use a 5 m detector, $\sim 90 \%$ of the neutrinos from pion decay are contained at $\sim 3 \mathrm{~km}$.

The optimal detector is a fine-grained calorimeter for electromagnetic shower reconstruction followed by a toroid muon spectrometer. This allows excellent reconstruction of the energy of the outgoing lepton from charged current events. We employ a Charm II style design [9, which uses a glass target calorimeter followed by a toroid. We assume one inch glass panels with active detectors interspersed for energy and position measurement. Glass provides an optimal choice of density, low enough to allow electromagnetic showers to be well sampled, but high enough that the detector length does not compromise acceptance for large angle muons by the toroid. Approximately $10 \%$ of the glass will be doped with scintillator to allow for background studies, as discussed in Sec. IIID.

The design introduces four identical sub-detectors of

| 600 M | $\nu_{\mu}$ CC Deep Inelastic Scattering |
| :---: | :---: |
| 190 M | $\nu_{\mu}$ NC Deep Inelastic Scattering |
| 75 k | $\nu_{\mu}$ electron NC elastic scatters (ES) |
| 700 k | $\nu_{\mu}$ electron CC quasi-elastic scatters (IMD) |
| 33 M | $\bar{\nu}_{\mu}$ CC Deep Inelastic Scattering |
| 12 M | $\bar{\nu}_{\mu}$ NC Deep Inelastic Scattering |
| 7 k | $\bar{\nu}_{\mu}$ electron NC elastic scatters (ES) |
| 0 k | $\bar{\nu}_{\mu}$ electron CC quasi-elastic scatters (WSIMD) |

TABLE I: Rates assumed for this paper. NC indicates "neutral current" and CC indicates "charged current."
this glass-calorimeter and toroid design, each a total of 29 m in length (including the toroid). Between each subdetector is a 15 m decay region for direct searches for new physics. The total fiducial volume is 3 ktons.

The NuSOnG run plan, for reasons discussed in Sec. IIIB and IIIC, concentrates on running in neutrino mode. This design will yield the rates shown in Table $\mathbb{I}$. These rates, before cuts, are assumed throughout the rest of the discussion. We can compare this sample to past experiments. The present highest statistics sample for $\nu_{\mu}$ and $\bar{\nu}_{\mu}$ ES is from CHARM II, with $2677 \pm 82$ events in neutrino mode and $2752 \pm 88$ events in antineutrino mode [5]. Thus the proposed experiment will have a factor of $30(2.5)$ more $\nu(\bar{\nu})$-electron events. As an example, after cuts, the first method of analysis described in Sec. IIID retains $63 \%$ of the $\nu$ sample. For deep inelastic scattering, 600 M and 190 M events are expected in neutrino and antineutrino modes, respectively. After minimal cuts to isolate DIS events [10], NuTeV had 1.62M DIS (NC+CC) events in neutrino mode and 0.35 M in antineutrino mode; thus NuSOnG has orders of magnitude more events.

The detector will incorporate several specialized regions. A region of fine vertex-tracking facilitates measurements of the strange sea relevant for the electroweak analysis, as described in ref. [2]. Two possibilities are under consideration: an emulsion detector or a silicon detector of the style of NOMAD-STAR [11]. Both are compact and easily accommodated. For further QCD studies, it will also be useful to intersperse alternative target materials: $\mathrm{C}, \mathrm{Al}, \mathrm{Fe}$, and $\mathrm{Pb}[2]$.

## III. ELECTROWEAK MEASUREMENTS IN NEUTRINO SCATTERING

Neutrino neutral current (NC) scattering is an ideal probe for new physics. An experiment like NuSOnG is unique in its ability to test the NC couplings by studying scattering of neutrinos from both electrons and quarks. A deviation from the Standard Model predictions in both the electron and quark measurements would present a compelling case for new physics.

The exchange of the $Z$ boson between the neutrino $\nu$
and fermion $f$ leads to the effective interaction:

$$
\begin{align*}
\mathcal{L}=-\sqrt{2} G_{F}[ & \left.\bar{\nu} \gamma_{\mu}\left(g_{V}^{\nu}-g_{A}^{\nu} \gamma_{5}\right) \nu\right]\left[\bar{f} \gamma^{\mu}\left(g_{V}^{f}-g_{A}^{f} \gamma_{5}\right) f\right] \\
=-\sqrt{2} G_{F}[ & \left.g_{L}^{\nu} \bar{\nu} \gamma_{\mu}\left(1-\gamma_{5}\right) \nu+g_{R}^{\nu} \bar{\nu} \gamma_{\mu}\left(1+\gamma_{5}\right) \nu\right] \\
& \times\left[g_{L}^{f} \bar{f} \gamma^{\mu}\left(1-\gamma_{5}\right) f+g_{R}^{f} \bar{f} \gamma^{\mu}\left(1+\gamma_{5}\right) f\right] \tag{2}
\end{align*}
$$

where the Standard Model values of the couplings are:

$$
\begin{align*}
g_{L}^{\nu} & =\sqrt{\rho}\left(+\frac{1}{2}\right) \\
g_{R}^{\nu} & =0 \\
g_{L}^{f} & =\sqrt{\rho}\left(I_{3}^{f}-Q^{f} \sin ^{2} \theta_{W}\right) \\
g_{R}^{f} & =\sqrt{\rho}\left(-Q^{f} \sin ^{2} \theta_{W}\right), \tag{3}
\end{align*}
$$

or equivalently,

$$
\begin{align*}
g_{V}^{\nu} & =g_{L}^{\nu}+g_{R}^{\nu}=\sqrt{\rho}\left(+\frac{1}{2}\right) \\
g_{A}^{\nu} & =g_{L}^{\nu}-g_{R}^{\nu}=\sqrt{\rho}\left(+\frac{1}{2}\right) \\
g_{V}^{f} & =g_{L}^{f}+g_{R}^{f}=\sqrt{\rho}\left(I_{3}^{f}-2 Q^{f} \sin ^{2} \theta_{W}\right) \\
g_{A}^{f} & =g_{L}^{f}-g_{R}^{f}=\sqrt{\rho}\left(I_{3}^{f}\right) \tag{4}
\end{align*}
$$

Here, $I_{3}^{f}$ and $Q^{f}$ are the weak isospin and electromagnetic charge of fermion $f$, respectively. In these formulas, $\rho$ is the relative coupling strength of the neutral to charged current interactions ( $\rho=1$ at tree level in the Standard Model). The weak mixing parameter, $\sin ^{2} \theta_{W}$, is related (at tree level) to $G_{F}, M_{Z}$ and $\alpha$ by

$$
\begin{equation*}
\sin ^{2} 2 \theta_{W}=\frac{4 \pi \alpha}{\sqrt{2} G_{F} M_{Z}^{2}} \tag{5}
\end{equation*}
$$

## A. Neutrino Electron Elastic Scattering

The differential cross section for $\nu_{\mu}$ and $\bar{\nu}_{\mu}$ ES, defined using the coupling constants described above, is:

$$
\begin{align*}
\frac{d \sigma}{d T}=\frac{2 G_{F}^{2} m_{e}}{\pi}[ & \left(g_{L}^{\nu} g_{V}^{e} \pm g_{L}^{\nu} g_{A}^{e}\right)^{2} \\
& +\left(g_{L}^{\nu} g_{V}^{e} \mp g_{L}^{\nu} g_{A}^{e}\right)^{2}\left(1-\frac{T}{E_{\nu}}\right)^{2} \\
& \left.-\left\{\left(g_{L}^{\nu} g_{V}^{e}\right)^{2}-\left(g_{L}^{\nu} g_{A}^{e}\right)^{2}\right\} \frac{m_{e} T}{E_{\nu}^{2}}\right] . \tag{6}
\end{align*}
$$

The upper and lower signs correspond to the neutrino and anti-neutrino cases, respectively. In this equation, $E_{\nu}$ is the incident $\nu_{\mu}$ energy and $T$ is the electron recoil kinetic energy.

More often in the literature, the cross section is defined in terms of the parameters $\left(g_{V}^{\nu e}, g_{A}^{\nu e}\right)$, which are defined as

$$
g_{V}^{\nu e} \equiv\left(2 g_{L}^{\nu} g_{V}^{e}\right)=\rho\left(-\frac{1}{2}+2 \sin ^{2} \theta_{W}\right)
$$

$$
\begin{equation*}
g_{A}^{\nu e} \equiv\left(2 g_{L}^{\nu} g_{A}^{e}\right)=\rho\left(-\frac{1}{2}\right) \tag{7}
\end{equation*}
$$

In terms of these parameters, we can write:

$$
\begin{align*}
\frac{d \sigma}{d T}= & \frac{G_{F}^{2} m_{e}}{2 \pi}\left[\left(g_{V}^{\nu e} \pm g_{A}^{\nu e}\right)^{2}\right. \\
& +\left(g_{V}^{\nu e} \mp g_{A}^{\nu e}\right)^{2}\left(1-\frac{T}{E_{\nu}}\right)^{2} \\
& \left.-\left\{\left(g_{V}^{\nu e}\right)^{2}-\left(g_{A}^{\nu e}\right)^{2}\right\} \frac{m_{e} T}{E_{\nu}^{2}}\right] . \tag{8}
\end{align*}
$$

When $m_{e} \ll E_{\nu}$, as is the case in NuSOnG, the third term in these expressions can be neglected. If we introduce the variable $y=T / E_{\nu}$, then

$$
\begin{equation*}
\frac{d \sigma}{d y}=\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi}\left[\left(g_{V}^{\nu e} \pm g_{A}^{\nu e}\right)^{2}+\left(g_{V}^{\nu e} \mp g_{A}^{\nu e}\right)^{2}(1-y)^{2}\right] \tag{9}
\end{equation*}
$$

Integrating, we obtain the total cross sections which are

$$
\begin{equation*}
\sigma=\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi}\left[\left(g_{V}^{\nu e} \pm g_{A}^{\nu e}\right)^{2}+\frac{1}{3}\left(g_{V}^{\nu e} \mp g_{A}^{\nu e}\right)^{2}\right] \tag{10}
\end{equation*}
$$

Note that

$$
\begin{align*}
\left(g_{V}^{\nu e}+g_{A}^{\nu e}\right)^{2} & =\rho^{2}\left(-1+2 \sin ^{2} \theta_{W}\right)^{2} \\
& =\rho^{2}\left(1-4 \sin ^{2} \theta_{W}+4 \sin ^{4} \theta_{W}\right) \\
\left(g_{V}^{\nu e}-g_{A}^{\nu e}\right)^{2} & =\rho^{2}\left(2 \sin ^{2} \theta_{W}\right)^{2} \\
& =\rho^{2}\left(4 \sin ^{4} \theta_{W}\right) \tag{11}
\end{align*}
$$

Therefore,

$$
\begin{align*}
& \sigma\left(\nu_{\mu} e\right)=\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi} \rho^{2}\left[1-4 \sin ^{2} \theta_{W}+\frac{16}{3} \sin ^{4} \theta_{W}\right] \\
& \sigma\left(\bar{\nu}_{\mu} e\right)=\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi} \frac{\rho^{2}}{3}\left[1-4 \sin ^{2} \theta_{W}+16 \sin ^{4} \theta_{W}\right] \tag{12}
\end{align*}
$$

The ratio of the integrated cross sections for neutrino to antineutrino electron ES is

$$
\begin{equation*}
R_{\nu / \bar{\nu}}=\frac{\sigma\left(\nu_{\mu} e\right)}{\left.\sigma^{( } \bar{\nu}_{\mu} e\right)}=3 \frac{1-4 \sin ^{2} \theta_{W}+\frac{16}{3} \sin ^{4} \theta_{W}}{1-4 \sin ^{2} \theta_{W}+16 \sin ^{4} \theta_{W}} \tag{13}
\end{equation*}
$$

Fig. 4 (top) shows the results for $\sin ^{2} \theta_{W}$ from many past experiments which have used this " $\nu / \bar{\nu} \mathrm{ES}$ ratio."

In the ratio, $R_{\nu / \bar{\nu}}$, the dependence on $\rho$ canceled. This directly extracts $\sin ^{2} \theta_{W}$. The relationship between the error on the ratio and the error on $\sin ^{2} \theta_{W}$, which for convenience we abbreviate as $z$, is:

$$
\begin{align*}
\delta z= & \left(\frac{32 z-12}{16 z^{2}-4 z+1}+\right. \\
& \left.\frac{448 z^{2}-144 z-512 z^{3}+12}{48 z^{2}-8 z-128 z^{3}+256 z^{4}+1}\right)^{-1} \delta R_{\nu / \bar{\nu}} \\
= & -0.103 \delta R_{\nu / \bar{\nu}}  \tag{14}\\
\delta z / z= & -0.575 \delta R_{\nu / \bar{\nu}} / R_{\nu / \bar{\nu}} \tag{15}
\end{align*}
$$



FIG. 4: Measurements of $\sin ^{2} \theta_{W}$ from past experiments. Top: neutrino-electron elastic scattering experiments. Bottom: neutrino DIS experiments. All DIS results are adjusted to the same charm mass (relevant for experiments not using the PW method). The Standard Model value, indicated by the line, is 0.2227 [12].
for $z=0.2227$ (or $R_{\nu / \bar{\nu}}=1.242$ ). Roughly, the fractional error on $\sin ^{2} \theta_{W}$ is $60 \%$ of the fractional error on $R_{\nu / \bar{\nu}}$.

## B. A New Technique: Normalization Through IMD

An experiment such as NuSOnG can make independent measurements of the electroweak parameters for both $\nu_{\mu}$ and $\bar{\nu}_{\mu}$-electron scattering. We can achieve this via ratios or by direct extraction of the cross section. In the case of $\nu_{\mu}$-electron scattering, we will use the ratio of the number of events in neutrino-electron elastic scattering to inverse muon decay:

$$
\begin{equation*}
\frac{N\left(\nu_{\mu} e^{-} \rightarrow \nu_{\mu} e^{-}\right)}{N\left(\nu_{\mu} e^{-} \rightarrow \mu^{-} \nu_{e}\right)}=\frac{\sigma_{N C}^{\nu e} \times \Phi^{\nu}}{\sigma^{I M D} \times \Phi^{\nu}} \tag{16}
\end{equation*}
$$

Because the cross section for IMD events is well determined by the Standard Model, this ratio should have low errors and will isolate the EW parameters from NC scattering. In the discussion below, we will assume that the systematic error on this ratio is $0.5 \%$.

In the case of $\bar{\nu}_{\mu}$ data, the absolute normalization is more complex because there is no equivalent process to inverse muon decay (since there are no positrons in the detector). One can use the fact that, for low exchange energy (or "nu") in Deep Inelastic Scattering,


FIG. 5: Kinematic distributions for IMD events from incident neutrino energy between 100 and 200 GeV . Left: $y$ distribution; right: $\theta_{\mu}$ distribution. Black: distribution of events before cuts; Red: distribution after cuts for analysis method 1 (see Sec. III D.
the cross sections in neutrino and antineutrino scattering approach the same constant, $A$ 13]. This is called the "low nu method" of flux extractions. For DIS events with low energy transfer and hence low hadronic en$\operatorname{ergy}\left(5 \lesssim E_{\text {had }} \lesssim 10 \mathrm{GeV}\right), N_{\nu D I S}^{\text {low } E_{\text {had }}}=\Phi^{\nu} A$ and $N_{\bar{\nu} D I S}^{\text {low } E_{h} a d}=\Phi^{\bar{\nu}} A$. The result is that the electroweak parameters can be extracted using the ratio

$$
\begin{equation*}
\frac{N_{\nu D I S}^{l o w} E_{\text {had }}}{N_{\bar{\nu} D I S}^{l o w} E_{\text {had }}} \times \frac{N\left(\bar{\nu}_{\mu} e^{-} \rightarrow \bar{\nu}_{\mu} e^{-}\right)}{N\left(\nu_{\mu} e^{-} \rightarrow \mu^{-} \nu_{e}\right)}=\frac{\Phi^{\nu}}{\Phi^{\bar{\nu}}} \times \frac{\sigma_{N C}^{\bar{\nu} e} \times \Phi^{\bar{\nu}}}{\sigma^{I M D} \times \Phi^{\nu}} . \tag{17}
\end{equation*}
$$

The first ratio cancels the DIS cross section, leaving the energy-integrated $\nu$ to $\bar{\nu}$ flux ratio. The IMD events in the denominator of the second term cancel the integrated $\nu$ flux. The NC elastic events cancel the integrated $\bar{\nu}$ flux.

Because of the added layer of complexity, the antineutrino ES measurement would have a higher systematic error than the neutrino ES scattering measurement. The potentially higher error is one factor leading to the plan that NuSOnG concentrate on neutrino running for the ES studies.

As shown in Fig. 2. IMD events have a kinematic threshold at 10.9 GeV . These events also have other interesting kinematic properties. The minimum energy of the outgoing muon in the lab frame is given by

$$
\begin{equation*}
E_{\mu l a b}^{\min }=\frac{m_{\mu}^{2}+m_{e}^{2}}{2 m_{e}}=10.9 \mathrm{GeV} \tag{18}
\end{equation*}
$$

In the detector described above, muons of this energy and higher will reach the toroid spectrometer without ranging-out in the glass. An interesting consequence is that, independent of $E_{\nu}$, the energy transfer in the interaction has a maximum value of

$$
\begin{equation*}
y_{\max }=1-\frac{10.9 \mathrm{GeV}}{E_{\nu}} \tag{19}
\end{equation*}
$$

Thus at low $E_{\nu}$, the cutoff in $y$ is less than unity, as shown in Fig. 5 (left). The direct consequence of this is


FIG. 6: Reconstructed neutrino energy (red) for IMD events before cuts compared to true neutrino energy (black).
a strong cutoff in angle of the outgoing muon, shown in Fig. 5 (right). In principle, one can reconstruct the full neutrino energy in these events:

$$
\begin{equation*}
E_{\nu}^{I M D}=\frac{1}{2} \frac{2 m_{e} E_{\mu}-m_{e}^{2}-m_{\mu}^{2}}{m_{e}-E_{\mu}+p_{\mu} \cos \theta_{\mu}} \tag{20}
\end{equation*}
$$

This formula depends on $\theta_{\mu}$, which is small. The reconstructed $E_{\nu}$ is smeared by resolution effects as seen in Fig. 6. While the analysis can be done by summing over all energies, these distributions indicate that an energy binned analysis may be possible. This is more powerful because one can fit for the energy dependence of backgrounds. For the illustrative analyzes below, however, we do not employ this technique.

The error on $\sin ^{2} \theta_{W}$ extracted from this ratio, $R_{E S / I M D}$, assuming a Standard Model value for $\rho$, is the same as the error on the ratio:

$$
\begin{equation*}
\frac{\delta\left(\sin ^{2} \theta_{W}\right)}{\sin ^{2} \theta_{W}} \approx \frac{\delta R_{E S / I M D}}{R_{E S / I M D}} \tag{21}
\end{equation*}
$$

Ref. [14] provides a useful summary of radiative corrections for the ES and IMD processes, which were originally calculated in Ref. [15]. The error from radiative corrections is expected to be below $0.1 \%$. It is noted that to reduce the error below $0.1 \%$, leading two-loop effects must be included. A new evaluation of the radiative corrections is underway [16].

## C. IMD Normalization vs. $\bar{\nu}$ Normalization

NuSOnG can measure both the $\nu / \bar{\nu}$ ES ratio, as in the case of past experiments shown in Eq. 13 , as well as the ES/IMD ratio. In the case of the former, to obtain the best measurement in a 5 year run, one would choose a 1:3 ratio of run time in $\nu$ versus $\bar{\nu}$ mode. In the latter case, one would maximize running in $\nu$ mode. The result of the two cases is a nearly equal error on $\sin ^{2} \theta_{W}$, despite the fact that the error on the $\nu / \bar{\nu} \mathrm{ES}$ is nearly twice that of the ES/IMD ratio. To understand this, compare Eq. (15) to Eq. 21. However, the ES/IMD ratio is substantially stronger for reasons of physics. Therefore, our conceptual design calls for running mainly with a $\nu$ beam. In this section we explore the issues for these two methods of measurement further. We also justify why the precision measurement requires high energies, only available from a Tevatron-based beam.

## 1. Comparison of the Two Measurement Options

From the point of view of physics, The ES/IMD ratio is more interesting than the $\nu / \bar{\nu} \mathrm{ES}$ ratio. This is because $\rho$ has canceled in the $\nu / \bar{\nu}$ ES ratio of Eq. (13), leaving the ratio insensitive to physics which manifests itself through changes in the NC coupling. Many of the unique physics goals of NuSOnG, discussed in Sec. IV, depend upon sensitivity to the NC coupling.

An equally important concern was one of systematics. The $\nu$ and $\bar{\nu}$ fluxes for a conventional neutrino beam are substantially different. For the case of NuSOnG, the fluxes are compared in Fig. 3. Predicting the differences in these fluxes from secondary production measurements and simulations leads to substantial systematic errors. For beams at high energies $(>30 \mathrm{GeV})$, such as $\mathrm{Nu}-$ SOnG, the "low nu" method [13] for determining the ratio of the neutrino to antineutrino fluxes from Deep Inelastic events, developed by CCFR and NuTeV and described in Sec. IIIB, can be employed. However, this leads to the criticism that one has introduced a new process into the purely-leptonic analysis.

Neither criticism is relevant to the ES/IMD ratio. The sensitivity to the new physics through the couplings does not cancel. Because both processes are in neutrino mode, the flux exactly cancels, as long as the neutrino energies are well above the IMD threshold (this will be illustrated in the analysis presented in Sec. IIID). This ratio has the added advantage of needing only neutrino-mode running,
which means that very high statistics can be obtained. This is clearly the more elegant solution.

It should be noted that nothing precludes continued running of NuSOnG beyond the 5 -year plan presented here. This run-length was selected as "reasonable" for first results. If interesting physics is observed in this first phase, an extended run in antineutrino mode may be warranted, in which case both the ES/IMD and $\nu / \bar{\nu}$ ES ratios could be measured. The latter would then constrain $\sin ^{2} \theta_{W}$ in a pure neutrino measurement and the former is then used to extract $\rho$.

To measure the ES/IMD ratio to high precision, there must be little low energy flux. This is because the IMD has a threshold of 10.9 GeV , and does not have substantial rate until $\sim 30 \mathrm{GeV}$. The low-energy cut-off in the flux (see Fig. 3) coming from the energy-angle correlation of neutrinos from pion decay, is ideal.

## 2. Why a Tevatron-based Beam is Best for Both Options

The ES/IMD measurement is not an option for the planned beams from the Main Injector at Fermilab. For both presently planned Main Injector experiments at Fermilab [17] and for the proposed Project-X DUSEL beam [18], the neutrino flux is peaked at $\sim 5 \mathrm{GeV}$. The majority of the flux of these beams is below 5 GeV , and most of the flux is below the 10.9 GeV IMD threshold. Because of this, one simply cannot use the IMD events to normalize.

In principle, the $\nu / \bar{\nu} \mathrm{ES}$ ratio could be used. However, in practice this will have large systematics. The $\nu$ and $\bar{\nu}$ fluxes for a horn beam are significantly different. First principles predictions of secondary mesons are not sufficient to reduce this error to the precision level. The energy range is well below the deep inelastic region where the "low nu" method can be applied to accurately extract a $\bar{\nu} / \nu$ flux ratio. Other processes, such as charged-current quasi-elastic scattering, could be considered for normalization, but the differences in nuclear effects in neutrino and antineutrino scattering for these events is not sufficiently well understood to yield a precision measurement.

Lastly, the ES rates for the present Main Injector beams are too low for a high statistics measurement. This is because the cross section falls linearly with energy. Event samples on the order of 10k may be possible with extended running in the Project X DUSEL beam in the future. From the point of view of statistics, even though two orders of magnitude more protons on target are supplied in such a beam, the Tevatron provides a substantially higher rate of ES per year of running.

Compared to the Main Injector beam, a Tevatronbased beam does not face these issues. The choice of running in neutrino mode provides the highest precision measurement while optimizing the physics.

| Quantity | Assumed Value | Uncertainty | Source of Estimate |
| :---: | :---: | :---: | :---: |
| Muon |  |  |  |
| Energy Resolution | $\delta E / E=10 \%$ | 2.5\% | NuTeV testbeam measurement |
| Energy Scale Error | $E_{\text {rec }}=1.0 \times E_{\text {true }}$ | 0.5\% | NuTeV testbeam measurement |
| Angular Resolution | $\delta \theta=0.011 / E^{0.96} \mathrm{rad}$ | 2.5\% | Multiple scattering fit simulation |
| Electron |  |  |  |
| Energy Resolution | $\delta E / E=0.23 / E^{0.5}$ | 1.0\% | Same as CHARM II |
| Energy Scale Error | $E_{\text {rec }}=1.0 \times E_{\text {true }}$ | 1.0\% | Scaled from CHARM II with NuSOnG statistics |
| Angular Resolution | $\delta \theta=0.008 / E^{0.5} \mathrm{rad}$ | 2.5\% | 2 better than CHARM II due to sampling |
| Flux |  |  |  |
| Normalization | 1.0 | $3 \%$ | Current total cross section uncertainty |
| Shape Uncertainty | 1.0 | 1\% | Similar to NuTeV low-nu method |
| Backgrounds |  |  |  |
| $\nu_{\mu} \mathrm{CCQE}$ | $1.0$ | 5\% | Extrapolated from NuTeV |
| $\nu_{e} \mathrm{CCQE}$ | 1.0 | $3 \%$ | Extrapolated from CHARM II |

TABLE II: Resolutions and systematic uncertainty estimates used in the parameterized Monte Carlo studies. The NuTeV estimates are based on Ref. [19] and the CHARM II estimates from Ref. 9]. Units for angles are radians and energies are in GeV .

## D. A $0.7 \%$ Measurement Goal for the ES to IMD Ratio

Achieving $0.7 \%$ precision on the ES/IMD measurement depends on reducing the backgrounds to an acceptable level without introducing significant systematics and while maintaining high signal statistics. Many of the systematic uncertainties will tend to cancel. The most important background for both the $\nu$-e neutral current and IMD events comes from charged current quasi-elastic (CCQE) scatters ( $\nu_{e} n \rightarrow p e$ and $\left.\nu_{\mu} n \rightarrow p \mu\right)$. These background CCQE processes have a much broader $Q^{2}$ as compared to the signal processes and, therefore, can be partially eliminated by kinematic cuts on the outgoing muon or electron. Initial cuts on the scattering angle and energy of the outgoing muon or electron can easily reduce the CCQE background by factors of 60 and 14 respectively while retaining over $50 \%$ of the $\nu-e$ neutral current and IMD signal. This leaves events with very forward scatters and outgoing scattered protons of low kinetic energy.

Because the NuSOnG design is at the conceptual stage and in order to be conservative, we have developed two different strategies for achieving a $0.7 \%$ error. This serves as a proof of principle that this level of error, or better, can be reached. The first method relies on detecting protons from the quasi-elastic scatter. The second method uses the beam kinematics to cut the low energy flux which reduces the CCQE background.

These methods were checked via two, independently written, parameterized Monte Carlos. The parameterized Monte Carlos made the assumptions given in Table II] where both the assumed values and uncertainties are presented. These estimates of resolutions and systematic errors are based on previous experimental measurements or on fits to simulated data. One Monte Carlo used the Nuance event generator 20 to produce events, while the other was an independently written event gen-
erator. Both Monte Carlos include nuclear absorption and binding effects.

The first strategy uses the number of protons which exit the glass to constrain the total rate of the background. In $\sim 33 \%$ of the events, a proton will exit the glass, enter a chamber and traverse the gas. This samples protons of all energies and $Q^{2}$, since the interactions occur uniformly throughout the glass. After initial cuts, the protons are below 100 MeV , and therefore highly ionizing. If we define 1 MIP as the energy deposited by a single minimum ionizing particle, like a muon, then the protons consistently deposit greater than 5 MIPs in the chamber. Thus, one can identify CCQE events by requiring $>4$ MIPS in the first chamber. The amount of remaining CCQE background after this requirement can be measured if a fraction such as $10 \%$ of the detector is made from scintillating glass that can directly identify CCQE events from light associated with the outgoing proton. A wide range of scintillating glasses have been developed 21 for nuclear experiments. These glasses are not commonly used in high energy physics experiments because the scintillation time constant is typically on the order of 100 ns . In a neutrino experiment, which has inherently lower rates than most particle experiments, this is not an issue. CCQE events can be identified by the scintillation light from the proton assuming reasonable parameters for the glass and readout photomultiplier tubes: 450 photons $/ \mathrm{MeV}$, an attenuation length of 2 m , eight phototubes per glass sheet, quantum efficiency of the tubes of $20 \%$. Using the identified CCQE events from the instrumented glass, the uncertainty in the residual background can be reduced to $2.0 \%$ for the IMD measurement. For the CCQE background to the $\nu_{\mu}-e$ neutral current measurement, the uncertainty is assumed to be $3 \%$ for the Monte Carlo prediction. Combining all the systematic errors leads to a $\sim 0.7 \%$ accuracy on the $\nu-e$ measurement as shown in Tab. III

In Tab. III, the cancellation of the flux errors should be
noted. This occurred because we use the ES/IMD ratio, as discussed in the previous section.

The second strategy involves reducing the relative CCQE background to signal by using a harder flux for the analysis. This study used the same Monte Carlos, with the resolutions listed in Tab. II, as the first analysis. The total systematic and statistical error achieved was $0.6 \%$. Below, we explain how a harder flux is obtained for the analysis. Then, we explain how this flux improves the signal-to-background in both the ES and IMD analyzes.

The strong correlation between energy and angle at the NuSOnG detector is used to isolate the harder flux. This is simplest to express in the non-bend view of the beamline, where it is given for pions by the well-known off-axis formula:

$$
\begin{equation*}
E_{\nu}=\frac{0.43 E_{\pi}}{1+\gamma^{2} \theta^{2}} \tag{22}
\end{equation*}
$$

where $\theta$ is the off-axis angle, $\gamma=E_{\pi} / m_{\pi}, E_{\pi}$ is the energy of the pion and $E_{\nu}$ is the energy of the neutrino. For the NuTeV beam and detector lay-out, this angle-energy dependence resulted in the sharp cutoff of the flux for $<30 \mathrm{GeV}$ shown in Fig. 3. Using the NuTeV G3 beam Monte Carlo [7], we have shown that by selecting vertices in the central region of the detector, one can adjust the energy where the flux sharply cuts off. Adjusting the aperture to retain flux above 50 GeV reduces the total event rate by $55 \%$.

A harder flux allows for background reduction in both the ES and the IMD samples while maintaining the signal at high efficiency. In the case of ES events, the background is from $\nu_{e}$ CCQE. The energy distribution of the electron is substantially different in the two cases. In the case of $\nu_{e}$ CCQE events, the electron carries most of the energy of the incoming neutrino because the exchange energy in the interaction is small. Thus the CCQE events produced by the harder flux populate the visible energy range above 50 GeV . On the other hand, the outgoing electron in ES events tends to populate the low visible energy region due to the combination of a flat $y$ distribution for the process convoluted with the incident neutrino energy spectrum. The result is that a cut on the visible energy less than 50 GeV reduces the error from the $\nu_{e}$ CCQE background to a negligible level. To understand the improvement in the IMD analysis, consider Fig. 2, which shows the threshold effects. The IMD signal is also rising with energy. In contrast, the $\nu_{\mu}$ CCQE rate, which is the most significant background, is flat with energy for fluxes above 1 GeV . This signal-to-background is greatly improved with a high energy flux. This allows looser cuts to be applied, which in turn reduces the systematics.

These two analyzes use substantially different strategies and can, in principle, be combined. Given these preliminary studies, we feel confident that as the detector moves from a conceptual to real design, we will be able to achieve a better than $0.7 \%$ error. However, for this paper we take the conservative approach of assuming $0.7 \%$.

## E. Neutrino Quark Scattering

Substantially higher precision has been obtained using neutrino-quark scattering, which compares neutralcurrent ( NC ) to charged-current (CC) scattering to extract $\sin ^{2} \theta_{W}$. However, these experiments are subject to issues of modeling in the quark sector. Fig. 4(bottom) reviews the history of these measurements.

The lowest systematic errors come from implementing a "Paschos-Wolfenstein style" [6] analysis. This PW technique would be used by any future experiment, including NuSOnG. This requires high purity $\nu$ and $\bar{\nu}$ beams, for which the following ratios of DIS events could be formed:

$$
\begin{align*}
R^{\nu} & =\frac{\sigma_{N C}^{\nu}}{\sigma_{C C}^{\nu}}  \tag{23}\\
R^{\bar{\nu}} & =\frac{\sigma_{N C}^{\bar{\nu}}}{\sigma_{C C}^{\bar{\nu}}} \tag{24}
\end{align*}
$$

Paschos and Wolfenstein [6] recast these as:

$$
\begin{equation*}
R^{-}=\frac{\sigma_{N C}^{\nu}-\sigma_{N C}^{\bar{\nu}}}{\sigma_{C C}^{\nu}-\sigma_{C C}^{\bar{\nu}}}=\frac{R^{\nu}-r R^{\bar{\nu}}}{1-r} \tag{25}
\end{equation*}
$$

where $r=\sigma_{C C}^{\bar{\nu}} / \sigma_{C C}^{\nu}$. In $R^{-}$many systematics cancel to first order, including the effects of the quark and antiquark seas for $u, d, s$, and $c$. Charm production only enters through $d_{\text {valence }}$ (which is Cabibbo suppressed) and at high $x$; thus the error from the charm mass is greatly reduced. The cross section ratios can be written in terms of the effective neutrino-quark coupling parameters $g_{L}^{2}$ and $g_{R}^{2}$ as

$$
\begin{align*}
R^{\nu} & =g_{L}^{2}+r g_{R}^{2}  \tag{26}\\
R^{\bar{\nu}} & =g_{L}^{2}+\frac{1}{r} g_{R}^{2}  \tag{27}\\
R^{-} & =g_{L}^{2}-g_{R}^{2}=\rho^{2}\left(\frac{1}{2}-\sin ^{2} \theta_{W}\right) \tag{28}
\end{align*}
$$

in which

$$
\begin{align*}
g_{L}^{2} & =\left(2 g_{L}^{\nu} g_{L}^{u}\right)^{2}+\left(2 g_{L}^{\nu} g_{L}^{d}\right)^{2} \\
& =\rho^{2}\left(\frac{1}{2}-\sin ^{2} \theta_{W}+\frac{5}{9} \sin ^{4} \theta_{W}\right)  \tag{29}\\
g_{R}^{2} & =\left(2 g_{L}^{\nu} g_{R}^{u}\right)^{2}+\left(2 g_{L}^{\nu} g_{R}^{d}\right)^{2} \\
& =\rho^{2}\left(\frac{5}{9} \sin ^{4} \theta_{W}\right) \tag{30}
\end{align*}
$$

In a variation on the PW idea, rather than directly form $R^{-}$, NuTeV fit simultaneously for $R^{\nu}$ and $R^{\bar{\nu}}$ to extract $\sin ^{2} \theta_{W}$, obtaining the value $\sin ^{2} \theta_{W}=0.2277 \pm$ 0.00162. Events were classified according to the length of hits in the scintillator planes of the NuTeV detector, with long events identified as CC interactions and short events as NC. An important background in the CC sample came from pion decay-in-flight, producing a muon in

|  | IMD Uncertainty | ES Uncertainty | Uncertainty on Ratio |
| :---: | :---: | :---: | :---: |
| Statistical Uncertainty | 0.18\% | 0.46\% | 0.49\% |
| Resolution Smearing |  |  |  |
| $\delta\left(\mathrm{E}_{\mu}\right)= \pm 2.5 \%$ | 0.00\% | 0.00\% | 0.00\% |
| $\delta\left(\theta_{\mu}\right)= \pm 2.5 \%$ | 0.04\% | 0.00\% | 0.04\% |
| $\delta\left(\mathrm{E}_{e}\right)= \pm 1.5 \%$ | 0.00\% | 0.01\% | 0.01\% |
| $\delta\left(\theta_{e}\right)= \pm 2.5 \%$ | 0.00\% | 0.09\% | 0.09\% |
| Energy Scale |  |  |  |
| $\delta\left(\right.$ Escale $\left._{\mu}\right)=0.5 \%$ | 0.37\% | 0.00\% | 0.37\% |
| $\delta\left(\right.$ Escale $\left._{e}\right)=1.5 \%$ | 0.00\% | 0.19\% | 0.19\% |
| Flux |  |  |  |
| Normalization | 3.00\% | 3.00\% | 0.00\% |
| High energy flux up 1\% | 0.25\% | 0.25\% | 0.00\% |
| Low energy flux up 1\% | 0.15\% | 0.13\% | 0.02\% |
| IMD Background: statistical error | 0.06\% | 0.00\% | 0.06\% |
| 2.0\% systematic error | 0.26\% | 0.00\% | 0.26\% |
| $\nu_{\mu}$ e Background: statistical error | 0.00\% | 0.12\% | 0.12\% |
| $3 \%$ systematic error | 0.00\% | 0.19\% | 0.19\% |
| Total Syst. Uncertainty on Ratio Total Stat. Uncertainty on Ratio Total Uncertainty on Ratio |  |  | 0.54\% |
|  |  |  | 0.51\% |
|  |  |  | 0.74\% |

TABLE III: Estimates of the IMD and ES uncertainties using a $>5$ MIP cut on the first downstream chamber. The columns give the errors for each process and then for the ratio. Errors are included for statistical uncertainties and uncertainties associated with the knowledge of resolution smearing, energy scale, flux shape, and backgrounds. The flux shape uncertainties are significantly reduced in the ratio measurement.
a NC shower. Significant backgrounds in the NC sample came from muons which ranged out or exited and from $\nu_{e}$ CC scatters which do not have a muon and thus are classified as "short."

In this paper, we present the sensitivity of NuSOnG to new physics if the NuTeV errors are reduced by a factor of $\sim 2$. This is a very conservative estimate, since most of the improvement comes from higher statistics. Only a $90 \%$ improvement in the systematics is required to reach this goal. Tab. IV argues why a $90 \%$ reduction in systematic error should be straightfroward to achieve. It is likely that the NuSOnG errors will be lower, but this requires detailed study.

In Table IV, we list the errors which NuTeV identified in their original analysis and indicate how NuSOnG will improve each error. Many of the largest experimental systematics of NuTeV are improved by introducing a fine-grained sampling calorimeter. The NuTeV detector had four inches of iron between unsegmented scintillator planes and eight inches between drift chamber planes. Better lateral segmentation and transverse detection will improve identification of scatters from intrinsic $\nu_{e} \mathrm{~s}$ in the beam and separation of CC and NC events by improved three-dimensional shower shape analyzes. The NuTeV analyzes of the intrinsic $\nu_{e}$ content [22] and the $\mathrm{CC} / \mathrm{NC}$ separation for the $\sin ^{2} \theta_{W}$ analysis which relied strictly on event length. With this said, the power of classifying by event length is shown by the fact that the NuTeV intrinsic $\nu_{e}$ analysis was sensitive to a discrepancy in the predicted intrinsic $\nu_{e}$ rate which was recently resolved with a new measurement of the $K_{e 3}$ branching ratio that
was published in 2003. Details of these issues are considered in the next section.

## F. The NuTeV Anomaly

From Fig. 4, it is apparent that the NuTeV measurement is in agreement with past neutrino scattering results, although these have much larger errors; however, in disagreement with the global fits to the electroweak data which give a Standard Model value of $\sin ^{2} \theta_{W}=0.2227$ [25]. Expressed in terms of the couplings, NuTeV measures:

$$
\begin{gather*}
g_{L}^{2}=0.30005 \pm 0.00137  \tag{31}\\
g_{R}^{2}=0.03076 \pm 0.00110 \tag{32}
\end{gather*}
$$

which can be compared to the Standard Model values of $g_{L}^{2}=0.3042$ and $g_{R}^{2}=0.0301$, respectively.

NuTeV is one of a set of $Q^{2} \ll m_{Z}^{2}$ experiments measuring $\sin ^{2} \theta_{W}$. It was performed at $Q^{2}=1$ to $140 \mathrm{GeV}^{2}$, $\left\langle Q_{\nu}^{2}\right\rangle=26 \mathrm{GeV}^{2},\left\langle Q_{\bar{\nu}}^{2}\right\rangle=15 \mathrm{GeV}^{2}$, which is also the expected range for NuSOnG. Two other precision low $Q^{2}$ measurements are from atomic parity violation [26] (APV), which samples $Q^{2} \sim 0$; and SLAC E158, a Møller scattering experiment at average $Q^{2}=0.026 \mathrm{GeV}^{2}$ [27]. Using the measurements at the $Z$-pole with $Q^{2}=M_{z}^{2}$ to fix the value of $\sin ^{2} \theta_{W}$, and evolving to low $Q^{2}[28]$, the APV and SLAC E158 are in agreement with the Standard Model. However, the radiative corrections to neutrino interactions allow sensitivity to high-mass par-

| Source | NuTeV <br> Error | Method of reduction in NuSOnG |
| :---: | :---: | :--- |
| Statistics | 0.00135 | Higher statistics |
| $\nu_{e}, \bar{\nu}_{e}$ flux prediction | 0.00039 | Improves in-situ measurement of $\bar{\nu}_{e}$ CC scatters, thereby constraining prediction, <br> due to better lateral segmentation and transverse detection. <br> Also, improved beam design to further reduce $\bar{\nu}_{e}$ from $K^{0}$. |
| Interaction vertex position | 0.00030 | Better lateral segmentation. |
| Shower length model | 0.00027 | Better lateral segmentation and transverse detection <br> will allow more sophisticated shower identification model. |
| Counter efficiency and noise | 0.00023 | Segmented scintillator strips of the type |
|  | 0.00018 | developed by MINOS [23] will improve this. |
| Enetter lateral segmentation. |  |  |
| Charm production, strange sea | 0.00047 | In-situ measurement [1, [2]. |
| $R_{L}$ | 0.00032 | In-situ measurement [1, [2]. |
| $\sigma^{\nu} / \sigma^{\nu}$ | 0.00022 | Likely to be at a similar level. |
| Higher Twist | 0.00014 | Recent results reduce this error [24. |
| Radiative Corrections | 0.00011 | New analysis underway, see text below. |
| Charm Sea | 0.00010 | Measured in-situ using wrong-sign muon production in DIS. |
| Non-isoscalar target | 0.00005 | Glass is isoscalar |

TABLE IV: Source and value of NuTeV errors on $\sin ^{2} \theta_{W}$, and reason why the error will be reduced in the PW-style analysis of NuSOnG. This paper assumes NuSOnG will reduce the total NuTeV error by a factor of two. This is achieved largerly through the improved statistical precision and requires only a $90 \%$ reduction in the overal NuTeV systematic error. This table argues that a better than $90 \%$ reduction is likely, but further study, once the detector design is complete, is required.
ticles which are complementary to the APV and Møllerscattering corrections. Thus, these results may not be in conflict with NuTeV. The NuSOnG measurement will provide valuable additional information on this question.

Since the NuTeV result was published, more than 300 papers have been written which cite this result. Several "Standard-Model" explanations have been suggested. While some constraints on these ideas can come from outside experiments, it will be necessary for any future neutrino scattering experiment, such as NuSOnG, to be able to directly address these proposed solutions. Also various Beyond Standard Model explanations have been put forward; those which best explain the result require a follow-up experiment which probes the neutral weak couplings specifically with neutrinos, such as NuSOnG. Here, we consider the explanations which are "within the Standard Model" and address the Beyond Standard Model later.

Several systematic adjustments to the NuTeV result have been identified since the result was published but have not yet been incorporated into a new NuTeV analysis. As discussed here, the corrections due to the two new inputs, a new $K_{e 3}$ branching ratio and a new strange sea symmetry, are significant in size but are in opposite direction - away and toward the Standard Model. So a re-analysis can be expected to yield a central value for NuTeV which will not change significantly. However, the error is expected to become larger.

In 2003, a new result from BNL865 [29] yielded a $K_{e 3}$ branching ratio which was $2.3 \sigma$ larger than past measurements and a value of $\left|V_{u s}\right|^{2}$ which brought the CKM matrix measurements into agreement with unitarity in


FIG. 7: Effect of various "Standard Model" explanations on the NuTeV anomaly. The $y$-axis is the deviation $\left(\delta \sin ^{2} \theta_{W}=\right.$ $\left.\sin ^{2} \theta_{W}^{S M}-\sin ^{2} \theta_{W}^{N u T e V}\right)$. The solid line is the published NuTeV deviation. Thick black lines extending from the NuTeV deviation show the range of possible pulls from NLO QCD and various isospin violation models. Note that the isospin violation models are mutually exclusive and so should not be added in quadrature. They are, from left to right, the full bag model, the meson cloud model, and the isospin QED model.
the first row 30. The measurement was confirmed by CERN NA48/2 [31]. The resulting increased $K_{e 3}$ branching ratio [12] increases the absolute prediction of intrinsic $\nu_{e} \mathrm{~s}$ in the NuTeV beam. This does not significantly change the error because the error on $K e 3$ was already included in the analysis. However, it introduces a correction moving the NuTeV result further away from the Standard Model, since it implies that in the original analysis, NuTeV under-subtracted the $\nu_{e}$ background in the NC sample. The shift in $\sin ^{2} \theta_{W}$ can be estimated in a back of envelope calculation to be about $\sim 0.001$ away from the Standard Model [32].

The final NuTeV measurement of the difference between the strange and anti-strange sea momentum distributions, was published in 2007 [33]. This "strange sea asymmetry" is defined as

$$
\begin{equation*}
x s^{-}(x) \equiv x s(x)-x \bar{s}(x) \tag{33}
\end{equation*}
$$

Because of mass suppression for the production of charm in CC scatters from strange quarks, a difference in the momentum distributions will result in a difference in the CC cross sections for neutrinos and antineutrinos. Thus a correction to the denominator of Eq. 25 would be required. The most recent next-to-leading order analysis finds the asymmetry, integrated over $x$ is $0.00195 \pm 0.00055 \pm 0.00138$ [33]. An integrated asymmetry of 0.007 is required to explain the published NuTeV result [33], and so one can estimate that this is a shift of about 0.0014 in $\sin ^{2} \theta_{W}$ toward the Standard Model. In this case, the errors on the NuTeV result will become larger because this effect was not originally considered in the analysis. A very naive estimate of the size of the increase can be derived by scaling the error on the integrated strange sea, quoted above, and is about 0.001 toward the Standard Model. If this naive estimate of the systematic error is borne out, then this could raise the NuTeV error on $\sin ^{2} \theta_{W}$ from 0.0016 to 0.0018 . NuSOnG will directly address the strange sea asymmetry in its QCD measurement program, as described in ref. [2].

In ref. [34, additional electromagnetic radiative corrections have been suggested as a source of the discrepancy. However, this paper only considered the effect of these corrections on $R^{\nu}$ and not $R^{\bar{\nu}}$ and for fixed beam energy of $E_{\nu}=80 \mathrm{GeV}$. The structure of the code from these authors has also made it difficult to modify for use in NuTeV . This has prompted a new set of calculations by other authors which are now under way [16]. There are, as yet, only estimates for the approximate size of newly identified effects, which are small.

The NuTeV analysis was not performed at a full NLO level in QCD; any new experiment, such as NuSOnG will need to undertake a full NLO analysis. This is possible given recently published calculations [35, 36, including those on target mass corrections 37. On Fig. 7, we show an early estimate of the expected size and direction of the pull [38]. On this plot, the solid horizontal line indicates the deviation of NuTeV from the Standard Model. The thick vertical lines, which emanate from the NuTeV
deviation, show the range of pulls estimated for various explanations. The range of pull for the NLO calculation is shown on the left.

The last possibility is that there is large isospin violation (or charge symmetry violation) in the nucleus. The NuTeV analysis assumed isospin symmetry, that is, $u(x)^{p}=d(x)^{n}$ and $d(x)^{p}=u(x)^{n}$. Isospin violation can come about from a variety of sources and is an interesting physics question in its own right. NuSOnG's direct constraints on isospin violation are discussed in ref. [2], which also considers the constraints from other experiments. Various models for isospin violation have been studied and their pulls range from less than $1 \sigma$ away from the Standard Model to $\sim 1 \sigma$ toward the Standard Model 39. We have chosen three examples 39] for illustration on Fig. 7 . the full bag model, the meson cloud model, and the isospin QED model. These are mutually exclusive models, so only one of these can affect the NuTeV anomaly.

## IV. THE TERASCALE PHYSICS REACH OF NUSONG

Even when new states are too heavy to be produced at resonance in collisions they can make their presence known indirectly, as virtual particles which affect SM processes through interference with SM contributions to amplitudes. The new heavy states induce small shifts in observables from SM predictions, and conversely precise measurements of these observables can constrain or detect new physics at mass scales well above the energies of the colliding particles. In this way the precision neutrino scattering measurements at NuSOnG will place TeV -scale indirect constraints on many classes of new physics, or perhaps detect new physics by measuring deviations from SM predictions. The effects of new high-scale physics may be reduced to a small number of effective operators along with corresponding parameters which may be fit to data. Although the particular set of operators used depends on broad assumptions about the new physics, the approach gives a parameterization of new physics which is largely model-independent.

For concreteness we will assume that NuSOnG will be able to measure the neutrino $\mathrm{ES} / \mathrm{IMD}$ ratio to a precision of $0.7 \%, \sigma\left(\bar{\nu}_{\mu} e\right)$ (normalized as per Sec. IIIB) to $1.3 \%$, and that NuSOnG will be able to halve the errors on NuTeV's measurement of DIS effective couplings, to $\Delta g_{L}^{2}=0.0007$ and $\Delta g_{R}^{2}=0.0006$ (where $g_{L}$ and $g_{R}$ were defined in Eqs. 29) and (30)).

We first parameterize new physics using the oblique parameters $S T$, which is appropriate when the important effects of the new physics appear in vacuum polarizations of gauge bosons. We next assume new physics effects manifest as higher-dimensional operators made of SM fermion fields. We separately consider the possibility that the gauge couplings to neutrinos are modified.

| Topic | Contribution of NuSOnG Measurement |
| :--- | :--- |
| Oblique Corrections | Four distinct and complementary probes of $S$ and $T$. <br>  <br> In the case of agreement with LEP/SLD: $\sim 25 \%$ improvement in electroweak precision. |
| Neutrino-lepton NSIs | Order of magnitude improvement in neutrino-electron effective couplings measurements. <br>  <br> Energy scale sensitivity up to $\sim 5 \mathrm{TeV}$ at $95 \%$ CL. |
| Neutrino-quark NSIs | Factor of two improvement in neutrino-quark effective coupling measurements. <br>  <br> Energy scale sensitivity up to $\sim 7 \mathrm{TeV}$ at $95 \%$ CL. |
| Mixing with Neutrissimos | $30 \%$ improvement on the $e$-family coupling in a global fit.  <br>  $75 \%$ improvement on the $\mu$-family coupling in a global fit. |
| Right-handed Couplings | Complementary sensitivity to $g_{R} / g_{L}$ compared to LEP. <br>  |

TABLE V: Summary of NuSOnG's contribution to general Terascale physics studies.

Realistic models usually introduce several new operators with relations among the coefficients; we consider several examples. A summary of the contributions of NuSOnG to the study of Terascale Physics is provided in Table V .

## A. Oblique corrections

For models of new physics in which the dominant loop corrections are vacuum polarization corrections to the $S U(2)_{L} \times U(1)_{Y}$ gauge boson propagators ("oblique" corrections), the $S T U$ (40, 41 parameterization provides a convenient framework in which to describe the effects of new physics on precision electroweak data. Differences between the predictions of a new physics model and those of a reference Standard Model (with a specified Higgs boson and top quark mass) can be expressed as nonzero values of the oblique correction parameters $S, T$ and $U . T$ and $U$ are sensitive to new physics that violates isospin, while $S$ is sensitive to isospin-conserving physics. Predictions of a Standard Model with Higgs or top masses different from the reference Standard Model may also be subsumed into shifts in $S$ and $T$ (in many models $U$ is much smaller than $S$ and $T$ and is largely unaffected by the Higgs mass, so it is often omitted in fits). Within a specific model of new physics the shift on the $S T$ plot away from the SM will be calculable [42. For example,

- A heavy Standard Model Higgs boson will make a positive contribution to $S$ and a larger negative contribution to $T$.
- Within the space of $Z^{\prime}$ models, a shift in almost any direction in $S T$ space is possible, with larger shifts for smaller $Z^{\prime}$ masses.
- Models with a fourth-generation of fermions will shift $S$ positive, and will shift $T$ positive if there are violations of isospin.

In constructing models incorporating several types of new physics the corresponding shifts to $S$ and $T$ combine; if contributions from different sectors are large, then they must conspire to cancel.


FIG. 8: The impact of NuSOnG on the limits of $S$ and $T$. The reference SM is $m_{t}=170.9 \mathrm{GeV}$, and $m_{H}=115 \mathrm{GeV}$. $1 \sigma$ bands due to NuSOnG observables are shown against the $90 \%$ contour from LEP/SLD. The central ellipses are the $68 \%$ and $90 \%$ confidence limit contours with NuSOnG included. See Eqs. 29) and 30 for the definitions of $g_{L}$ and $g_{R}$.

The constraints on $S$ and $T$ from the full set of precision electroweak data strongly restrict the models of new physics which are viable. The strongest constraints are from LEP/SLD, which give a current bound of

$$
\begin{align*}
S & =-0.02 \pm 0.11 \\
T & =+0.06 \pm 0.13 \\
\operatorname{Corr}(S, T) & =0.91 \tag{34}
\end{align*}
$$

The ES and DIS measurements from NuSOnG provide four distinct and complementary probes of $S$ and $T$, as shown in Fig. 8. If the target precision is achieved, and assuming the NuSOnG agree with SM predictions, NuSOnG will further reduce the errors on $S$ and $T$ from the LEP/SLD values to

$$
\begin{aligned}
& S=-0.05 \pm 0.09 \\
& T=+0.02 \pm 0.10
\end{aligned}
$$

$$
\begin{equation*}
\operatorname{Corr}(S, T)=0.87 \tag{35}
\end{equation*}
$$

The $\sim 25 \%$ reduction in the errors is primarily due to the improved measurement of $g_{L}^{2}$. We note that the error $g_{L}^{2}$ is likely to be further reduced (see Sec. IIIE), and so the this is conservative estimate of NuSOnG's contribution to the physics.

## B. Non-standard interactions

NuSOnG will probe new physics that modifies neutrino-quark and neutrino-electron scattering. If the masses associated to the new degrees of freedom are much larger than the center of mass energy $\left(s=2 m_{e} E_{\text {beam }} \lesssim\right.$ $0.5 \mathrm{GeV}^{2}$ ) then modifications to these processes are welldescribed by higher-dimensional effective operators. In the context of neutrino reactions, these operators are also referred to as non-standard interactions (NSI's). In a model-independent effective Lagrangian approach these effective operators are added to the SM effective Lagrangian with arbitrary coefficients. Expressions for experimental observables can be computed using the new effective Lagrangian, and the arbitrary coefficients can then be constrained by fitting to data. Typically, bounds on the magnitude of the coefficients are obtained using only one or a few of the available effective operators. This approach simplifies the analysis and gives an indication of the scale of constraints, although we must be mindful of relationships among different operators that will be imposed by specific assumptions regarding the underlying physics.

To assess the sensitivity of NuSOnG to "heavy" new physics in neutral current processes, we introduce the following effective Lagrangian for neutrino-fermion interactions [44, 48, 49]:

$$
\begin{align*}
\mathcal{L}_{\mathrm{NSI}}=-\sqrt{2} G_{F}\left[\bar{\nu}_{\alpha} \gamma_{\sigma} P_{L} \nu_{\beta}\right] & {\left[\varepsilon_{\alpha \beta}^{f V} \bar{f} \gamma^{\sigma} f-\varepsilon_{\alpha \beta}^{f A} \bar{f} \gamma^{\sigma} \gamma_{5} f\right] } \\
=-2 \sqrt{2} G_{F}\left[\bar{\nu}_{\alpha} \gamma_{\sigma} P_{L} \nu_{\beta}\right][ & {\left[\varepsilon_{\alpha \beta}^{f L} \bar{f} \gamma^{\sigma} P_{L} f\right.} \\
& \left.+\varepsilon_{\alpha \beta}^{f R} \bar{f} \gamma^{\sigma} P_{R} f\right] . \tag{36}
\end{align*}
$$

where $\alpha, \beta=e, \mu, \tau$ and $L, R$ represent left-chiral and right-chiral fermion fields. If $\alpha \neq \beta$, then the $\alpha \leftrightarrow \beta$ terms must be Hermitian conjugates of each other, i.e. $\varepsilon_{\beta \alpha}=\varepsilon_{\alpha \beta}^{*}$. NuSOnG is sensitive to the $\beta=\mu$ couplings. This effective Lagrangian is appropriate for parameterizing corrections to neutral current processes; an analysis of corrections to charged-current processes requires a different set of four-fermion operators.

Assuming $\varepsilon_{\alpha \beta}=0$ for $\alpha \neq \beta$ we need consider only the terms $\varepsilon_{\mu \mu}^{f *}(*=V, A, L, R)$. If we rewrite Eq. (2) as

$$
\begin{align*}
\mathcal{L}=-\sqrt{2} G_{F}\left[\bar{\nu} \gamma_{\mu} P_{L} \nu\right] & {\left[g_{V}^{\nu f} \bar{f} \gamma^{\mu} f-g_{A}^{\nu f} \bar{f} \gamma^{\mu} \gamma_{5} f\right] } \\
=-2 \sqrt{2} G_{F}\left[\bar{\nu} \gamma_{\mu} P_{L} \nu\right][ & {\left[g_{L}^{\nu f} \bar{f} \gamma^{\mu} P_{L} f\right.} \\
& \left.+g_{R}^{\nu f} \bar{f} \gamma^{\mu} P_{R} f\right] \tag{37}
\end{align*}
$$

where

$$
\begin{align*}
g_{V}^{\nu f} & =2 g_{L}^{\nu} g_{V}^{f}=\rho\left(I_{3}^{f}-2 Q^{f} \sin ^{2} \theta_{W}\right) \\
g_{A}^{\nu f} & =2 g_{L}^{\nu} g_{A}^{f}=\rho\left(I_{3}^{f}\right) \\
g_{L}^{\nu f} & =2 g_{L}^{\nu} g_{L}^{f}=\rho\left(I_{3}^{f}-Q^{f} \sin ^{2} \theta_{W}\right) \\
g_{R}^{\nu f} & =2 g_{L}^{\nu} g_{R}^{f}=\rho\left(-Q^{f} \sin ^{2} \theta_{W}\right) \tag{38}
\end{align*}
$$

then we see that adding Eq. (36) to the SM Lagrangian will simply shift the effective couplings:

$$
\begin{align*}
g_{V}^{\nu f} \longrightarrow \tilde{g}_{V}^{\nu f} & =g_{V}^{\nu f}+\varepsilon_{\mu \mu}^{f V} \\
g_{A}^{\nu f} \longrightarrow \tilde{g}_{A}^{\nu f} & =g_{A}^{\nu f}+\varepsilon_{\mu \mu}^{f A} \\
g_{L}^{\nu f} \longrightarrow \tilde{g}_{L}^{\nu f} & =g_{L}^{\nu f}+\varepsilon_{\mu \mu}^{f L} \\
g_{R}^{\nu f} \longrightarrow \tilde{g}_{R}^{\nu f} & =g_{R}^{\nu f}+\varepsilon_{\mu \mu}^{f R} \tag{39}
\end{align*}
$$

Consequently, errors on the $g_{P}^{\nu f}$,s translate directly into errors on the $\varepsilon_{\mu \mu}^{f P}$ 's, $P=V, A$ or $P=L, R$.

## 1. Neutrino-lepton NSI

A useful review of present constraints on non-standard neutrino-electron interactions can be found in ref. 45]. As this paper states, and as we show below, an improved measurement of neutrino-elecron scattering is needed.

The world average value for neutrino-electron effective couplings, dominated by CHARM II, is

$$
\begin{align*}
g_{V}^{\nu e} & =-0.040 \pm 0.015 \\
g_{A}^{\nu e} & =-0.507 \pm 0.014 \\
\operatorname{Corr}\left(g_{V}^{\nu e}, g_{A}^{\nu e}\right) & =-0.05 \tag{40}
\end{align*}
$$

The current $1 \sigma$ bounds from CHARM II, Eq. 40) translates to $\left|\varepsilon_{\mu \mu}^{e P}\right|<0.01,(P=L, R)$ with a correlation of 0.07 [44]. At the current precision goals, NuSOnG's $\nu_{\mu} e$ and $\bar{\nu}_{\mu} e$ will significantly reduce the uncertainties on these NSI's, to

$$
\begin{align*}
\left|\varepsilon_{\mu \mu}^{e V}\right| & <0.0036, \\
\left|\varepsilon_{\mu \mu}^{e A}\right| & <0.0019, \\
\operatorname{Corr}\left(\varepsilon_{\mu \mu}^{e V}, \varepsilon_{\mu \mu}^{e A}\right) & =-0.57, \tag{41}
\end{align*}
$$

or in terms of the chiral couplings,

$$
\begin{align*}
\left|\varepsilon_{\mu \mu}^{e L}\right| & <0.0015, \\
\left|\varepsilon_{\mu \mu}^{e R}\right| & <0.0025, \\
\operatorname{Corr}\left(\varepsilon_{\mu \mu}^{e L}, \varepsilon_{\mu \mu}^{e R}\right) & =0.64 . \tag{42}
\end{align*}
$$

Even in the absence of a $\sigma\left(\bar{\nu}_{\mu} e\right)$ measurement $\varepsilon_{\mu \mu}^{e L}$ and $\varepsilon_{\mu \mu}^{e R}$ can be constrained from the $\nu_{\mu} e$ scattering data alone through a fit to the recoil electron energy spectrum (see Eq. (9).

We first consider the constraint on $\varepsilon_{\mu \mu}^{e L}$ and $\varepsilon_{\mu \mu}^{e R}$ from the total cross section $\sigma\left(\nu_{\mu} e\right)$. It is convenient to recast the effective interaction slightly, as

$$
\begin{align*}
\mathcal{L}_{\mathrm{NSI}}^{e} & =-2 \sqrt{2} G_{F}\left[\bar{\nu}_{\alpha} \gamma_{\sigma} P_{L} \nu_{\mu}\right]\left[\varepsilon_{\alpha \mu}^{e L} \bar{e} \gamma^{\sigma} P_{L} e+\varepsilon_{\alpha \mu}^{e R} \bar{e} \gamma^{\sigma} P_{R} e\right] \\
& =+\frac{\sqrt{2}}{\Lambda^{2}}\left[\bar{\nu}_{\alpha} \gamma_{\sigma} P_{L} \nu_{\mu}\right]\left[\cos \theta \bar{e} \gamma^{\sigma} P_{L} e+\sin \theta \bar{e} \gamma^{\sigma} P_{R} e\right] \tag{43}
\end{align*}
$$

The new physics is parameterized by two coefficients $\Lambda$ and $\theta . \Lambda$ represents the broadly-defined new physics scale while $\theta \in[0,2 \pi]$ defines the relative coupling of left-chiral and right-chiral electrons to the new physics. As an example, a scenario with a purely "left-handed" $Z^{\prime}$ that couples to leptons with coupling $g^{\prime}$ would be described by $\Lambda \propto M_{Z^{\prime}} / g^{\prime}$ and $\theta=0$ or $\theta=\pi$, depending on the relative sign between $g^{\prime}$ and the electroweak couplings. $\Lambda$ and $\theta$ are related to to the NSI parameters in Eq. (36) by

$$
\begin{equation*}
\varepsilon_{\alpha \mu}^{e L}=-\frac{\cos \theta}{2 G_{F} \Lambda^{2}}, \quad \varepsilon_{\alpha \mu}^{e R}=-\frac{\sin \theta}{2 G_{F} \Lambda^{2}} . \tag{44}
\end{equation*}
$$

Note that we have generalized from our assumption of the previous section and not taken $\alpha=\mu$ necessarily. At NuSOnG, new physics modifies (pseudo)elastic neutrinoelectron scattering. Here we use the word "pseudo" to refer to the fact that we cannot identify the flavor of the final-state neutrino, which could be different from the incoming neutrino flavor in the case of flavor changing neutral currents.

The shift in the total cross section is

$$
\begin{align*}
\frac{\delta \sigma\left(\nu_{\mu} e\right)}{\sigma\left(\nu_{\mu} e\right)}= & \frac{\left\{2 g_{L}^{\nu e} \varepsilon_{\mu \mu}^{e L}+\left(\varepsilon_{\mu \mu}^{e L}\right)^{2}\right\}+\frac{1}{3}\left\{2 g_{R}^{\nu e} \varepsilon_{\mu \mu}^{e R}+\left(\varepsilon_{\mu \mu}^{e R}\right)^{2}\right\}}{\left(g_{L}^{\nu e}\right)^{2}+\frac{1}{3}\left(g_{R}^{\nu e}\right)^{2}} \\
\approx & -\left(\frac{516 \mathrm{GeV}}{\Lambda}\right)^{2} \cos (\theta-\phi) \\
& +0.096\left(\frac{516 \mathrm{GeV}}{\Lambda}\right)^{4}\left(1+2 \cos ^{2} \theta\right) \tag{45}
\end{align*}
$$

where

$$
\begin{equation*}
\tan \phi=\frac{g_{R}^{\nu e}}{3 g_{L}^{\nu e}} \approx-0.28 \tag{46}
\end{equation*}
$$

When $\mathcal{O}\left(\varepsilon^{2}\right)$ terms are negligible, a $0.7 \%$ measurement of $\sigma\left(\nu_{\mu} e\right)$ translates into a $95 \%$ confidence level bound of

$$
\begin{equation*}
\Lambda>(4.4 \mathrm{TeV}) \times \sqrt{|\cos (\theta-\phi)|} \tag{47}
\end{equation*}
$$

from elastic scattering.
The measurement of the electron recoil energy will allow us to do better. Fig. 9(dark line) depicts the $95 \%$ confidence level sensitivity of NuSOnG to the physics described by Eq. (43) when $\nu_{\alpha}=\nu_{\mu}$, obtained after fitting the recoil electron kinetic energy distribution. Fig. 9 (closed contour) represents how well NuSOnG should be able to measure $\Lambda$ and $\theta$, at the $95 \%$ level. Weaker bounds from pseudoelastic scattering are also shown. We have not included "data" from $\bar{\nu}_{\mu}$-electron


FIG. 9: (DARK LINES) $95 \%$ confidence level sensitivity of NuSOnG to new heavy physics described by Eq. 43) when $\nu_{\alpha}=\nu_{\mu}$ (higher curve) and $\nu_{\alpha} \neq \nu_{\mu}$ (lower curve). (CLOSED CONTOURS) NuSOnG measurement of $\Lambda$ and $\theta$, at the $95 \%$ level, assuming $\nu_{\alpha}=\nu_{\mu}, \Lambda=3.5 \mathrm{TeV}$ and $\theta=2 \pi / 3$ (higher, solid contour) and $\nu_{\alpha} \neq \nu_{\mu}, \Lambda=1 \mathrm{TeV}$ and $\theta=4 \pi / 3$ (lower, dashed contour). Note that in the pseudoelastic scattering case $\left(\nu_{\alpha} \neq \nu_{\mu}\right) \theta$ and $\pi+\theta$ are physically indistinguishable.
scattering. While there will be fewer of these events, they should qualitatively improve our ability to pin down the new physics parameters given the distinct dependency on $g_{V}^{\nu e}$ and $g_{A}^{\nu e}$ (see Sec. III A).

Eq. (43) does not include all effective dimension-six operators that contribute to neutrino-electron (pseudo) elastic scattering. All neglected terms will either not contribute at NuSOnG, or were assumed to be suppressed with respect to Eq. 43). In turn, terms proportional to a right-handed neutrino current $\bar{\nu}_{R} \gamma_{\sigma} \nu_{R}$ lead to negligibly small effects since neutrino masses are negligibly small and we are dealing with neutrino beams produced by pion and muon decay (i.e., for all practical purposes, we have a purely left-handed muon neutrino beam and a purely right-handed muon antineutrino beam). Chirality violating effective operators (e.g. $\left(\bar{\nu}_{R} \nu_{L}\right)\left(\bar{e}_{L} e_{R}\right)$ ), on the other hand, are expected to be suppressed with respect to Eq. (43) by terms proportional to neutrino masses and the electron mass (measured in units of $\Lambda$ ). The reason is that, in the limit of massless neutrinos or a massless electron, chiral symmetry is restored while such operators explicitly violate it. For the same reason, dimension-five magnetic moment-type operators ( $\bar{\nu} \sigma_{\rho \sigma} \nu F^{\rho \sigma}$ ) have also been neglected.

We note also that Eq. (43) violates $S U(2)_{L}$ unless one also includes similar terms where $\nu_{L} \leftrightarrow \ell_{L}(\ell=$ $e, \mu, \tau)$. In this case, certain flavor combinations would be
severely constrained by electron-electron scattering and rare muon and tau decays. One way around such constraints is to postulate that the operators in Eq. (43) are dimension-eight operators proportional to $\bar{L} H^{*} \gamma_{\sigma} L H$, where $L$ is the left-chiral lepton doublet and $H$ is the Higgs scalar doublet. In this case, $1 / \Lambda^{2}$ should be replaced by $v^{2} / \Lambda^{4}$, where $v=246 \mathrm{GeV}$ is the scale of electroweak symmetry breaking.

Finally, another concern is whether modifications to the charged current neutrino-electron (pseudo)quasielastic scattering ((pseudo)IMD, $\left.\nu_{\mu} e \rightarrow \nu_{\alpha} \mu\right)$ can render the translation of NuSOnG data into constraints or measurements of $\theta$ and $\Lambda$ less straightforward. This turns out not to be the case, since new physics contributions to $\nu_{\mu} e \rightarrow \nu_{\alpha} \mu$ are already very well constrained by precision studies of muon decay. Hence, given the provisos of the two previous paragraph, Eq. 43) is expected to capture all "heavy" new physics effects in (pseudo)elastic neutrino electron scattering.

## 2. Neutrino-quark NSI

We next consider the $f=u, d$ case. The change in the parameters $g_{L}^{2}$ and $g_{R}^{2}$ (see Eqs. 2930 ) due to the NSI's is

$$
\begin{align*}
\Delta g_{L}^{2} & =2 g_{L}^{\nu u} \varepsilon_{\mu \mu}^{u L}+2 g_{L}^{\nu d} \varepsilon_{\mu \mu}^{d L} \\
& \approx+0.69 \varepsilon_{\mu \mu}^{u L}-0.85 \varepsilon_{\mu \mu}^{d L} \\
\Delta g_{R}^{2} & =2 g_{R}^{\nu u} \varepsilon_{\mu \mu}^{u R}+2 g_{R}^{\nu d} \varepsilon_{\mu \mu}^{d R} \\
& \approx-0.31 \varepsilon_{\mu \mu}^{u R}+0.15 \varepsilon_{\mu \mu}^{d R} . \tag{48}
\end{align*}
$$

so only these linear combinations are constrained. The bounds from NuTeV (rescaled to $1 \sigma$ bounds from ref. (44) are:

$$
\begin{align*}
\varepsilon_{\mu \mu}^{u L} & =-0.0053 \pm 0.0020 \\
\varepsilon_{\mu \mu}^{d L} & =+0.0043 \pm 0.0016 \\
\left|\varepsilon_{\mu \mu}^{u R}\right| & <0.0035 \\
\left|\varepsilon_{\mu \mu}^{d R}\right| & <0.0073 \tag{49}
\end{align*}
$$

These bounds are obtained by setting only one of the parameters be non-zero at a time. If NuSOnG reduces the errors on the NuTeV measurement of $g_{L}^{2}$ and $g_{R}^{2}$ by a factor of 2 , the $1 \sigma$ bounds on the NSI parameters are similarly reduced:

$$
\begin{align*}
\left|\varepsilon_{\mu \mu}^{u L}\right| & <0.001 \\
\left|\varepsilon_{\mu \mu}^{d L}\right| & <0.0008 \\
\left|\varepsilon_{\mu \mu}^{u R}\right| & <0.002 \\
\left|\varepsilon_{\mu \mu}^{d R}\right| & <0.004 \tag{50}
\end{align*}
$$

In terms of a new physics scale defined as $\Lambda=1 / \sqrt{2 \mathrm{G}_{\mathrm{F}}} \varepsilon$, these constraints range from $\Lambda>3 \mathrm{TeV}$ to $\Lambda>7 \mathrm{TeV}$.

We note that neutrino-quark scattering will also be sensitive to NSIs which correct CC interactions. These interactions are not included in Eq. (36). If they are
important, as is the case in some of the scenarios we treat later, a new analysis is necessary and the bounds above cannot be used. This is to be contrasted to the neutrinolepton case, discussed in the previous subsection.

## C. Neutrissimos, Neutrino Mixing and Gauge Couplings



FIG. 10: Potential constraint on $\epsilon_{e}$ and $\epsilon_{\mu}$ from NuSOnG (see Eq. 55). This is a two-dimensional projection of a 4 parameter fit with $S, T, \epsilon_{e}$ and $\epsilon_{\mu}$. The green ellipse is the $90 \%$ CL contour of a fit to all the charge current particle decay data + LEP/SLD.

In those classes of models which include moderately heavy electroweak gauge singlet ("neutrissimo") states, with masses above 45 GeV , the mixing of the $S U(2)_{L^{-}}$ active neutrinos and the sterile states may lead to a suppression of the neutrino-gauge couplings. The resulting pattern of modified interactions is distinct from those of the previous section since they will also induce correlated shifts to the charged-current coupling. For example, Ref. 46] presents models with one sterile state per active neutrino flavor and intergenerational mixing among neutrinos. In these models the flavor eigenstates are linear combinations of mass eigenstates, and those mass eigenstates too heavy to be produced in final states result in an effective suppression of the neutrino-gauge boson coupling. This suppression may be flavor-dependent depending on the structure of the neutrino mixing matrix. If the mass matrix contains Majorana terms, such models permit both lepton flavor violation and lepton universality violation.

Neutrinos couple to the $W$ and the $Z$ through interactions described by:

$$
\mathcal{L}=\frac{g}{\sqrt{2}} W_{\mu}^{-} \bar{\ell}_{L} \gamma^{\mu} \nu_{\ell L}+\frac{g}{\sqrt{2}} W_{\mu}^{+} \bar{\nu}_{\ell L} \gamma^{\mu} \ell_{L}
$$

$$
\begin{equation*}
+\frac{e}{2 s c} Z_{\mu} \bar{\nu}_{\ell L} \gamma^{\mu} \nu_{\ell L} \tag{51}
\end{equation*}
$$

where $\ell=e, \mu, \tau$. If the neutrinos mix with gauge singlet states so that the $S U(2)_{L}$ interaction eigenstate is a superposition of mass eigenstates $\nu_{\ell, \text { light }}$ and $\nu_{\ell, \text { heavy }}$

$$
\begin{equation*}
\nu_{\ell L}=\nu_{\ell, \text { light }} \cos \theta_{\ell}+\nu_{\ell, \text { heavy }} \sin \theta_{\ell} \tag{52}
\end{equation*}
$$

then the interaction of the light states is given by

$$
\begin{align*}
\mathcal{L} & \left.\overline{\overline{ }} g W_{\mu}^{-} \bar{\ell}_{L} \gamma^{\mu} \nu_{\ell, \text { light }}+\frac{g}{\sqrt{2}} W_{\mu}^{+} \bar{\nu}_{\ell, \text { light }} \gamma^{\mu} \ell_{L}\right) \cos \theta_{\ell} \\
& (53)  \tag{53}\\
& +\left(\frac{e}{2 s c} Z_{\mu} \bar{\nu}_{\ell, \text { light }} \gamma^{\mu} \nu_{\ell, \text { light }}\right) \cos ^{2} \theta_{\ell}
\end{align*}
$$

Defining

$$
\begin{equation*}
\epsilon_{\ell} \equiv 1-\cos ^{2} \theta_{\ell} \tag{54}
\end{equation*}
$$

the shift in the Lagrangian due to this mixing is

$$
\begin{align*}
\delta \mathcal{L} & =-\left(\frac{g}{\sqrt{2}} W_{\mu}^{-} \bar{\ell}_{L} \gamma^{\mu} \nu_{\ell}+\frac{g}{\sqrt{2}} W_{\mu}^{+} \bar{\nu}_{\ell} \gamma^{\mu} \ell_{L}\right) \frac{\epsilon_{\ell}}{2} \\
& -\left(\frac{e}{2 s c} Z_{\mu} \bar{\nu}_{\ell} \gamma^{\mu} \nu_{\ell}\right) \epsilon_{\ell} \tag{55}
\end{align*}
$$

where we have dropped the subscript "light" from the neutrino fields.

Lepton universality data from $W$ decays and from charged current $\pi, \tau$ and $K$ decays [47] constraint differences $\epsilon_{\ell_{i}}-\epsilon_{\ell_{j}}$. LEP/SLD and other precision electroweak data will imposed additional constraints on $\epsilon_{\ell}$ in combination with the oblique parameters, as will NuSOnG. A fit to all the charge current decay data and LEP/SLD with $S, T, \epsilon_{e}$ and $\epsilon_{\mu}$ yields

$$
\begin{align*}
S & =-0.05 \pm 0.11 \\
T & =-0.44 \pm 0.28 \\
\epsilon_{e} & =0.0049 \pm 0.0022 \\
\epsilon_{\mu} & =0.0023 \pm 0.0021 \tag{56}
\end{align*}
$$

If we now included hypothetical data from NuSOnG, assuming NuSOnG achieves its precision goals and measures central values consistent with the Standard Model, we see the constraints on $\epsilon_{\mu}$ and $\epsilon_{e}$ are substantially improved. In this case, the fit yields

$$
\begin{align*}
S & =0.00 \pm 0.10 \\
T & =-0.11 \pm 0.12 \\
\epsilon_{e} & =0.0030 \pm 0.0017 \\
\epsilon_{\mu} & =0.0001 \pm 0.0012 \tag{57}
\end{align*}
$$

Fig. 10 shows the two dimensional cross section in the $\epsilon_{e}-\epsilon_{\mu}$ plane of the four dimensional fit. The likelihood coutours are 2 D projections. Though not obvious from the figure, it is NuSOnG's improved measurement of $g_{L}^{2}$ which contributes the most to strengthening the bounds on the $\epsilon_{\ell}$.

In models of this class lepton flavor violating decays such as $\mu \rightarrow e \gamma$ impose additional constraints on products $\epsilon_{\ell_{i}} \epsilon_{\ell_{j}}$. For example, the strong constraint from
$\mu \rightarrow e \gamma$ implies $\epsilon_{e} \epsilon_{\mu} \approx 0$. This type of model has been proposed as a solution to the NuTeV anomaly. If we take take only one of $\epsilon_{e}$ or $\epsilon_{\mu}$ to be nonzero (to respect the constraint from $\mu \rightarrow e \gamma$ ), the NuTeV value of $g_{L}^{2}$ is accommodated in the fit by best-fit values of $\epsilon$ that are large and positive and best-fit values of T are large and negative (consistent with a heavy Higgs).

## D. Right-handed coupling of the neutrino to the $Z$

In the Standard Model, neutrino couplings to the $W$ and $Z$-bosons are purely left-handed. The fact that the neutrino coupling to the $W$-boson and an electron is purely left-handed is, experimentally, a well-established fact (evidence includes precision measurements of pion and muon decay, nuclear processes, etc.). By contrast, the nature of the neutrino coupling to the $Z$ boson is, experimentally, far from being precisely established 50 . The possibility of a right-handed neutrino- $Z$-boson coupling is not included in the previous discussions, and is pursued separately in this subsection.

The best measurement of the neutrino coupling to the $Z$-boson is provided by indirect measurements of the invisible $Z$-boson width at LEP. In units where the Standard Model neutrino- $Z$-boson couplings are $g_{L}^{\nu}=0.5$, $g_{R}^{\nu} \equiv 0$, the LEP measurement [51] translates into $\left(g_{L}^{\nu}\right)^{2}+\left(g_{R}^{\nu}\right)^{2}=0.2487 \pm 0.0010$. Note that this result places no meaningful bound on $g_{R}^{\nu}$.

Precise, model-independent information on $g_{L}^{\nu}$ can be obtained by combining $\nu_{\mu}+e$ scattering data from CHARM II and LEP and SLD data. Assuming modelindependent couplings of the fermions to the $Z$-boson, $\nu_{\mu}+e$ scattering measures $g_{L}^{\nu}=\sqrt{\rho} / 2$, while LEP and SLD measure the left and right-handed couplings of the electron to the $Z$. The CHARM II result translates into $\left|g_{L}^{\nu}\right|=0.502 \pm 0.017$ [50], assuming that the chargedcurrent weak interactions produce only left-handed neutrinos. In spite of the good precision of the CHARM II result (around 3.5\%), a combination of all available data allows $\left|g_{R}^{\nu} / g_{L}^{\nu}\right| \sim 0.4$ at the two $\sigma$ confidence level 50.

Significant improvement in our understanding of $g_{R}^{\nu}$ can only be obtained with more precise measurements of $\nu+e$ scattering, or with the advent of a new high intensity $e^{+} e^{-}$collider, such as the ILC. By combining ILC running at the $Z$-boson pole mass and at $\sqrt{s}=170 \mathrm{GeV}$, $\left|g_{R}^{\nu} / g_{L}^{\nu}\right| \lesssim 0.3$ could be constrained at the two $\sigma$ level after analyzing $e^{+} e^{-} \rightarrow \gamma+$ missing energy events 50].

Assuming that $g_{L}^{\nu}$ can be measured with $0.7 \%$ uncertainty, Fig. 11 depicts an estimate of how precisely $g_{R}^{\nu}$ could be constrained once NuSOnG "data" is combined with LEP data. Fig. 11 (left) considers the hypothesis that the Standard Model expectations are correct. In this case, NuSOnG data would reveal that $g_{R} / g_{L}$ is less than 0.2 at the two sigma level. On the other hand, if $g_{R} / g_{L}=0.25-$ in good agreement with the current CHARM II and LEP data - NuSOnG data should reveal that $g_{R} \neq 0$ at more than the two sigma level, as depicted


FIG. 11: Precision with which the right-handed neutrino- $Z$-boson coupling can be determined by combining NuSOnG measurements of $g_{L}^{\nu}$ with the indirect determination of the invisible $Z$-boson width at LEP if (left) the $\nu+e$ scattering measurement is consistent with the Standard Model prediction $g_{L}^{\nu}=0.5$ and (right) the $\nu+e$ scattering measurement is significantly lower, $g_{L}^{\nu}=0.485$, but still in agreement with the CHARM II measurement(at the one sigma level). Contours (black, red) are one and two sigma, respectively. The star indicates the Standard Model expectation.
in Fig. 11(right).
The capability of performing this measurement in other experiments has been examined. The NuSOnG measurement compares favorably, and complements, the ILC capabilities estimated in [50]. Ref [52] studied measurements using other neutrino beams, including reactor fluxes and beta beams. NuSOnG's reach is equivalent to or exceeds the most optimistic estimates for these various neutrino sources.

## V. SPECIFIC THEORETICAL MODELS AND EXPERIMENTAL SCENARIOS

If NuSOnG's measurements agree with the SM within errors, we will place stringent constraints on new physics models; if they disagree, it will be a signal for new physics. In the latter case the availability of both DIS and ES channels will improve our ability to discriminate among new physics candidates. NuSOnG will also provide an important complement to the LHC. The LHC will provide detailed information about the spectrum of new states directly produced. However, measurements of the widths of these new states will provide only limited information about their couplings. NuSOnG will probe in multiple ways the couplings of these new states to neutrinos and to other SM particles.

In this section we provide several case studies of NuSOnG sensitivity to specific models of new physics. These include several typical $Z^{\prime}$ models, leptoquark models, models of R-parity violating supersymmetry, and models with extended Higgs sectors. We examine how
these will affect $\nu_{\mu} e$ ES and $\nu_{\mu} N$ DIS at tree-level. Our list is far from exhaustive but serves to illustrate the possibilities. We summarize our contributions in Table V

The opposite way to approach this problem is to ask: in the face of evidence for new Terascale Physics, how can we differentiate between specific models? NuSOnG has the potential to discover new physics through indirect probes, in the event that one or more of its measurements definitively contradicts SM predictions. We discuss several possible patterns of deviation of modelindependent parameters from SM predictions and some interpretations in terms of particular models. This is presented in the context of various expectations for LHC to illustrate how NuSOnG enhances the overall physics program. Since the NuTeV reanalysis is ongoing, and since the ES constraints from CHARM-II are weak, it is prudent that we commit to no strong assumptions about the central value of the NuSOnG measurements but instead consider all reasonable outcomes.

## A. Sensitivity in the Case of Specific Theoretical Models

We next consider the constraints imposed by the proposed NuSOnG measurements on explicit models of BSM physics. An explicit model provides relations among effective operators which give stronger and sometimes better-motivated constraints on new physics than is obtained from bounds obtained by considering effective op-

| Model | Contribution of NuSOnG Measurement |
| :---: | :--- |
| Typical $Z^{\prime}$ Choices: $(B-x L),(q-x u),(d+x u)$ | At the level of, and complementary to, LEP II bounds. |
| Extended Higgs Sector | At the level of, and complementary to $\tau$ decay bounds. |
| R-parity Violating SUSY | Sensitivity to masses $\sim 2 \mathrm{TeV}$ at $95 \%$ CL. <br> Improves bounds on slepton couplings by $\sim 30 \%$ and <br> on some squark couplings by factors of 3-5. |
| Intergenerational Leptoquarks with non-degenerate masses | Accesses unique combinations of couplings. <br> Also accesses coupling combinations explored by $\pi$ decay bounds, <br> at a similar level. |

TABLE VI: Summary of NuSOnG's contribution in the case of specific models


FIG. 12: Some examples of NuSOnG's $2 \sigma$ sensitivity to new high-mass particles commonly considered in the literature. For explanation of these ranges, and further examples, see text.
erators one by one, but at the expense of the generality of the conclusions. Many models can be analyzed using the effective Lagrangian of Eq. (36), but others introduce new operators and must be treated individually. The list of models considered is not exhaustive, but rather illustrates the new physics reach of NuSOnG.

## 1. $Z^{\prime}$ models

Massive $Z^{\prime}$ fields are one of the simplest signatures of physics beyond the Standard Model. (For a recent review, see [53].) $Z^{\prime}$ vector bosons are generic in grand unified theories and prevalent in theories that address the electroweak gauge hierarchy. They may stabilize the weak scale directly by canceling off quadratic divergences of Standard Model fields, as in theories of extradimensions or Little Higgs theories. In supersymmetric models, $Z^{\prime}$ fields are not needed to cancel quadratic divergences, but are still often tied to the scale of softbreaking (and hence the electroweak scale). In these last two cases, the $Z^{\prime}$ typically has a TeV -scale mass, and is an attractive target for NuSOnG.

|  | $U(1)_{B-x L}$ | $U(1)_{q+x u}$ | $U(1)_{10+x \overline{5}}$ | $U(1)_{d-x u}$ |
| :---: | :---: | :---: | :---: | :---: |
| $\nu_{\mu L}, e_{L}$ | $-x$ | -1 | $x / 3$ | $(-1+x) / 3$ |
| $e_{R}$ | $-x$ | $-(2+x) / 3$ | $-1 / 3$ | $x / 3$ |

TABLE VII: Charges of $\nu_{\mu L}, e_{L}, e_{R}$ under 4 phenomenologically viable classes of $U(1)^{\prime}$ symmetries. Each value of $x$ corresponds to a different $U(1)^{\prime}$ symmetry that is considered.

If the $Z^{\prime}$ mass is sufficiently large, its exchange is welldescribed at NuSOnG energies by the effective operator of Eq. 43). In this case, the new physics scale is related to the $Z^{\prime}$ model by $\Lambda \sim M_{Z^{\prime}} / g_{Z^{\prime}}$, the ratio of the $Z^{\prime}$ mass to its gauge-coupling. Further model-dependence shows up in the ratio of fermion charges under the $\mathrm{U}(1)^{\prime}$ symmetry associated with the $Z^{\prime}$, and the presence of any $Z-Z^{\prime}$ mixing. With reasonable theoretical assumptions, the absence of new sources of large flavor-changing neutral currents, the consistency of Yukawa interactions, and anomaly cancellation with a minimal number of exotic fermions, the number of interesting models can be reduced substantially, to four discrete families of generic $U(1)^{\prime}$ models each containing one free parameter, $x$ [54]. In Table V A 1 we indicate the charges of $\nu_{\mu L}, e_{L}, e_{R}$ under these families of $U(1)^{\prime}$ symmetries.

Using the sensitivity of NuSOnG to the scale $\Lambda$ in $\nu_{\mu}$ scattering shown in Figure 9, we can bound the combination $M_{Z^{\prime}} / g_{Z^{\prime}}$ for the four families of $Z^{\prime}$ models as a function of $x$. It is important to note that these bounds are competitive with the LEP-II bounds found in [54], which are based on $Z^{\prime}$ decays to all fermions, not just electrons and neutrinos.

There are $Z^{\prime}$ models which distinguish among generations can affect neutrino scattering. These will be probed by NuSOnG at the TeV scale [55, 56, 57, 58, 59]. Among these, $B-3 L_{\mu}$ was suggested as a possible explanation for the NuTeV anomaly [60, 61, however, we show here that this is not the case. Nevertheless, it remains an interesting example to consider.

In the gauged $B-3 L_{\mu}$ the $Z^{\prime}$ modifies $\nu_{\mu} N$ DIS. The exchange of the $Z^{\prime}$ between the $\nu_{\mu}$ and the quarks induces operators with coefficients

$$
\varepsilon_{\mu \mu}^{u L}=\varepsilon_{\mu \mu}^{u R}=\varepsilon_{\mu \mu}^{d L}=\varepsilon_{\mu \mu}^{d R}
$$



FIG. 13: $95 \%$ confidence level sensitivity of NuSOnG to the indicated $Z^{\prime}$ models. The charges of the electrons and neutrinos under the underlying $U(1)^{\prime}$ gauge symmetry are described in Table VA 1 The bounds are plotted as functions of the parameter $x$, which scans over allowed fermion charges for each family of $U(1)^{\prime}$ symmetries, versus the ratio $M_{z^{\prime}} / g_{Z^{\prime}}$.

$$
\begin{equation*}
=-\frac{1}{2 \sqrt{2} G_{F}} \frac{g_{Z^{\prime}}^{2}}{M_{Z^{\prime}}^{2}} \equiv \varepsilon_{B-3 L_{\mu}} \tag{58}
\end{equation*}
$$

which shift $g_{L}^{2}$ and $g_{R}^{2}$ by

$$
\begin{equation*}
\Delta g_{L}^{2}=\Delta g_{R}^{2}=-\frac{2 s^{2}}{3} \varepsilon_{B-3 L_{\mu}} \tag{59}
\end{equation*}
$$

It should be noted that since $\varepsilon_{B-3 L_{\mu}}$ is negative, this shows that both $g_{L}^{2}$ and $g_{R}^{2}$ will be shifted positive. This, in fact, excludes gauged $B-3 L_{\mu}$ as an explanation of the NuTeV anomaly. With this said, a NuSOnG measurement of $g_{L}^{2}$ and $g_{R}^{2}$ that improves on NuTeV errors by a factor of 2 yields a $2 \sigma$ bound

$$
\begin{equation*}
\frac{M_{Z^{\prime}}}{g_{Z^{\prime}}}>2.2 \mathrm{TeV} \tag{60}
\end{equation*}
$$

which is comparable and complementary to the existing bound from D0, and thus interesting to consider.

## 2. Models with extended Higgs sectors

In the Zee 62] and Babu-Zee 63] models, an isosinglet scalar $h^{+}$with hypercharge $Y=+1$ is introduced, which couples to left-handed lepton doublets $\ell$ as

$$
\begin{equation*}
\mathcal{L}_{h}=\lambda_{a b}\left(\overline{\ell_{a L}^{c}} i \sigma_{2} \ell_{b L}\right) h^{+}+h . c . \tag{61}
\end{equation*}
$$

where $(a b)$ are flavor indices: $a, b=e, \mu, \tau$. The exchange of a charged Higgs induces the effective operator from

Eq. (36) which with coefficient

$$
\begin{equation*}
\varepsilon_{\mu \mu}^{e L}=-\frac{1}{\sqrt{2} G_{F}} \frac{\left|\lambda_{e \mu}\right|^{2}}{M_{h}^{2}}, \quad \varepsilon_{\mu \mu}^{e R}=0 \tag{62}
\end{equation*}
$$

From Eq. 42, the $95 \%$ bound is:

$$
\begin{equation*}
\frac{M_{h}}{\left|\lambda_{e \mu}\right|}>5.2 \mathrm{TeV} \tag{63}
\end{equation*}
$$

competitive with current bound from $\tau$-decay of 5.4 TeV.

## 3. $R$-parity violating SUSY

Assuming the particle content of the Minimal Supersymmetric Standard Model (MSSM), the most general Rparity violating superpotential (involving only tri-linear couplings) has the form 64]

$$
\begin{equation*}
W_{R}=\frac{1}{2} \lambda_{i j k} \hat{L}_{i} \hat{L}_{j} \hat{E}_{k}+\lambda_{i j k}^{\prime} \hat{L}_{i} \hat{Q}_{j} \hat{D}_{k}+\frac{1}{2} \lambda_{i j k}^{\prime \prime} \hat{U}_{i} \hat{D}_{j} \hat{D}_{k} \tag{64}
\end{equation*}
$$

where $\hat{L}_{i}, \hat{E}_{i}, \hat{Q}_{i}, \hat{D}_{i}$, and $\hat{U}_{i}$ are the left-handed MSSM superfields defined in the usual fashion, and the subscripts $i, j, k=1,2,3$ are the generation indices. $S U(2)_{L}$ gauge invariance requires the couplings $\lambda_{i j k}$ to be antisymmetric in the first two indices:

$$
\begin{equation*}
\lambda_{i j k}=-\lambda_{j i k} \tag{65}
\end{equation*}
$$

The purely baryonic operator $\hat{U}_{i} \hat{D}_{j} \hat{D}_{k}$ is irrelevant to neutrino scattering, so only the $9 \lambda_{i j k}$ and $27 \lambda_{i j k}^{\prime}$ couplings are of interest.

From the $\hat{L} \hat{L} \hat{E}$ part of the Eq. 64 slepton exchange will contribute to $\nu_{\mu} e \mathrm{ES}$ at NuSOnG. These induce fourfermion operators appearing in Eq. (36) with corresponding coefficients

$$
\begin{align*}
\varepsilon_{\mu \mu}^{e L} & =-\frac{1}{4 \sqrt{2} G_{F}} \sum_{k=1}^{3} \frac{\left|\lambda_{21 k}\right|^{2}}{M_{\tilde{e}_{k R}}^{2}} \\
\varepsilon_{\mu \mu}^{e R} & =+\frac{1}{4 \sqrt{2} G_{F}} \sum_{j=1,3} \frac{\left|\lambda_{2 j 1}\right|^{2}}{M_{\tilde{e}_{j L}}^{2}} \tag{66}
\end{align*}
$$

If we place bounds on the sleptons one at a time, then Eq. (42) translates to the $2 \sigma$ bounds shown in TableVIII, presented for masses of 100 GeV . To rescale to different masses, use $\left(\frac{M}{100 \mathrm{GeV}}\right)$. This can be compared to current bounds Ref. 65]. NuSOnG improves all of these bounds.

From the $\hat{L} \hat{Q} \hat{D}$ part of Eq. 64, squark exchange will contribute to contribute to NC $\nu_{\mu} N$ DIS and CC $\nu_{\mu} N$ DIS. The resulting shifts in $g_{L}^{2}$ and $g_{R}^{2}$ are

$$
\begin{align*}
\delta g_{L}^{2} & =2\left[g_{L}^{\nu d} \varepsilon_{\mu \mu}^{d L}-g_{L}^{2} \varepsilon_{c}\right] \\
\delta g_{R}^{2} & =2\left[g_{R}^{\nu d} \varepsilon_{\mu \mu}^{d R}-g_{R}^{2} \varepsilon_{c}\right] \tag{67}
\end{align*}
$$

where

$$
\varepsilon_{\mu \mu}^{d L}=-\frac{1}{4 \sqrt{2} G_{F}} \sum_{k=1}^{3} \frac{\left|\lambda_{21 k}^{\prime}\right|^{2}}{M_{\tilde{d}_{k R}}^{2}}
$$

| Coupling | 95\% NuSOnG bound | lurrent $95 \%$ bound |
| :---: | :---: | :--- |
| $\left\|\lambda_{121}\right\|$ | 0.03 | $0.05\left(V_{u d}\right)$ |
| $\left\|\lambda_{122}\right\|$ | 0.04 | $0.05\left(V_{u d}\right)$ |
| $\left\|\lambda_{123}\right\|$ | 0.04 | $0.05\left(V_{u d}\right)$ |
| $\left\|\lambda_{231}\right\|$ | 0.05 | $0.07(\tau$ decay $)$ |
| $\left\|\lambda_{21}^{\prime}\right\|$ | 0.05 | $0.06(\pi$ decay $)$ |
| $\left\|\lambda_{212}^{\prime}\right\|$ | 0.06 | $0.06(\pi$ decay $)$ |
| $\left\|\lambda_{213}^{\prime}\right\|$ | 0.06 | $0.06(\pi$ decay $)$ |
| $\left\|\lambda_{221}^{\prime}\right\|$ | 0.07 | $0.21(D$ meson decay $)$ |
| $\left\|\lambda_{231}^{\prime}\right\|$ | 0.07 | $0.45\left(Z \rightarrow \mu^{+} \mu^{-}\right)$ |

TABLE VIII: Potential bounds on the R-parity violating $L L E$ (top) and $L Q D$ (bottom) couplings from NuSOnG, assuming that only one coupling is non-zero at a time for each set. All squark and slepton masses are set to 100 GeV . To obtain limits for different masses, rescale by $\left(\frac{M}{100 \mathrm{GeV}}\right)$. Current bounds are from Ref. 65].

$$
\begin{align*}
\varepsilon_{\mu \mu}^{d R} & =-\frac{1}{4 \sqrt{2} G_{F}} \sum_{j=1}^{3} \frac{\left|\lambda_{2 j 1}^{\prime}\right|^{2}}{M_{\tilde{d}_{j L}}^{2}} \\
\varepsilon_{c} & =+\frac{1}{4 \sqrt{2} G_{F}} \sum_{k=1}^{3} \frac{\left|\lambda_{21 k}^{\prime}\right|^{2}}{M_{\tilde{d}_{k R}}^{2}}=-\varepsilon_{\mu \mu}^{d L} \tag{68}
\end{align*}
$$

$\varepsilon_{\mu \mu}^{d L}$ and $\varepsilon_{\mu \mu}^{d R}$ are associated with terms of Eq. 36p, while $\varepsilon_{c}$ is associated with a four-fermion interaction that corrects charged currents,

$$
\begin{equation*}
-2 \sqrt{2} G_{F} \varepsilon_{c}\left[\left(\overline{\mu_{L}} \gamma_{\sigma} \nu_{\mu L}\right)\left(\overline{u_{L}} \gamma^{\sigma} d_{L}\right)+h . c .\right] . \tag{69}
\end{equation*}
$$

The shifts in $g_{L}^{2}$ and $g_{R}^{2}$ are:

$$
\begin{align*}
\delta g_{L}^{2} & =2\left(g_{L}^{\nu d}+g_{L}^{2}\right) \varepsilon_{\mu \mu}^{d L} \\
\delta g_{R}^{2} & =2 g_{R}^{2} \varepsilon_{\mu \mu}^{d L}+2 g_{R}^{\nu d} \varepsilon_{\mu \mu}^{d R} \tag{70}
\end{align*}
$$

Assuming the projected precision goals for NuSOnG on $g_{L}^{2}$ and $g_{R}^{2}$, and allowing only one of the couplings to be nonozero at a time, the $2 \sigma$ bounds are given in TableVIII mass of 100 GeV , in all cases. To obtain limits for different masses, one simply rescales by $\left(\frac{M}{100 \mathrm{GeV}}\right)$. NuSOnG's measurements are competitive with $\pi$ decay bounds, and improves the current bounds on the 221 and 231 couplings by factors of 3 and 5 , respectively.

## 4. Intergenerational leptoquark models

Measurements of $g_{L}^{2}$ and $g_{R}^{2}$ are sensitive to leptoquarks. Because the exchange of a leptoquark can interfere with both $W$ and $Z$ exchange processes, we cannot use the limits on the NSI's of Eq. (36), since we must also include the effects of the four-fermion operators associated with charged-current processes. Instead, the interactions of leptoquarks with ordinary matter can be described in a model-independent fashion by an effective low-energy Lagrangian as discussed in Refs. 66, 68 for generation-universal leptoquark couplings. For leptoquarks to contribute to $\nu_{\mu} N$ DIS, they must couple second generation leptons to first generation quarks, so we
use the more general Lagrangian of 67, 69, which allows the coupling constants to depend on the generations of the quarks and leptons that couple to each leptoquark. We summarize the quantum numbers and couplings of the various leptoquarks fields in Table IX, our notation conventions are those of Ref. 69.

The four-fermion operators induced by leptoquark exchange will affect NC and/or CC processes, and at NuSOnG the effect manifests itself in shifts $g_{L}^{2}$ and $g_{R}^{2}$. Assuming degenerate masses within each iso-multiplet, the shifts in $g_{L}^{2}$ and $g_{R}^{2}$ can be written generically as

$$
\begin{align*}
& \delta g_{L}^{2}=C_{L} \frac{\left|\lambda_{L Q}^{12}\right|^{2} / M_{L Q}^{2}}{g^{2} / M_{W}^{2}}=\frac{C_{L}}{4 \sqrt{2} G_{F}} \frac{\left|\lambda_{L Q}^{12}\right|^{2}}{M_{L Q}^{2}} \\
& \delta g_{R}^{2}=C_{R} \frac{\left|\lambda_{L Q}^{12}\right|^{2} / M_{L Q}^{2}}{g^{2} / M_{W}^{2}}=\frac{C_{R}}{4 \sqrt{2} G_{F}} \frac{\left|\lambda_{L Q}^{12}\right|^{2}}{M_{L Q}^{2}} \tag{71}
\end{align*}
$$

where $\lambda_{L Q}^{12}$ denotes the $(i j)=(12)$ coupling of the leptoquark and $M_{L Q}$ is its mass. In table $X$ we list what they are, and in figure 14 we plot the dependence of $\delta g_{L}^{2}$ and $\delta g_{R}^{2}$ on the ratio $\left|\lambda_{L Q}\right|^{2} / M_{L Q}^{2}$. Table X also lists the projected NuSOnG bounds on the coupling constants [70]. Existing bounds on $S_{1}, \vec{S}_{3}, V_{1}$, and $\vec{V}_{3}$ couplings from $R_{\pi}=\operatorname{Br}(\pi \rightarrow e \nu) / \operatorname{Br}(\pi \rightarrow \mu \nu)$ are already much stronger, but could be circumvented for $\vec{S}_{3}$ and $\vec{V}_{3}$ if the masses within the multiplet are allowed to be non-degenerate.

## B. Interplay with LHC to Isolate the Source of New Physics

By the time NuSOnG runs, the LHC will have accumulated a wealth of data and will have begun to change the particle physics landscape. The message from LHC data may be difficult to decipher, however. As discussed below, NuSOnG will be able to help elucidate the new physics revealed at the LHC. The discovery of a Higgs along with the anticipated measurement of the top mass to 1 GeV precision would effectively fix the center of the $S T$ plot and will enhance the power of the precision electroweak data as a tool for discovering new physics. If additional resonances are discovered at the LHC, it is still likely that little will be learned about their couplings.

The NuSOnG experiment provides complementary information to LHC. Rather than generalize, to illustrate the power of NuSOnG, two specific examples are given here. We emphasize that these are just two of a wide range of examples, but they serve well to demonstrate the point. Here we have chosen examples from typical new physics models other than $Z^{\prime}$ models which were discussed above, in order to demonstrate the physics range which can be probed by NuSOnG.

| Leptoquark |  | Spin | F | $S U(3)_{C}$ | $I_{3}$ | $Y$ | $Q_{\text {em }}$ | Allowed Couplings |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $S_{1}$ | $S_{1}^{0}$ | 0 | -2 | 3 | 0 | $\frac{1}{3}$ | $\frac{1}{3}$ | $g_{1 L}\left(\overline{u_{L}^{c}} e_{L}-\overline{d_{L}^{c}} \nu_{L}\right), g_{1 R}\left(\overline{u_{R}^{c}} e_{R}\right)$ |
| $\tilde{S}_{1}$ | $\tilde{S}_{1}^{0}$ | 0 | -2 | 3 | 0 | $\frac{4}{3}$ | 4 | $\tilde{g}_{1 R}\left(\overline{d_{R}^{c}} e_{R}\right)$ |
| $V_{2 \mu}$ | $\begin{aligned} & V_{2 \mu}^{+} \\ & V_{2 \mu}^{-} \end{aligned}$ | 1 | -2 | $\overline{3}$ | $\begin{aligned} & +\frac{1}{2} \\ & -\frac{1}{2} \end{aligned}$ | $\frac{5}{6}$ | $\frac{4}{3}$ <br> $\frac{1}{3}$ | $\begin{aligned} & g_{2 L}\left(\overline{\bar{d}_{R}^{c}} \gamma^{\mu} e_{L}\right), g_{2 R}\left(\overline{d_{L}^{c}} \gamma^{\mu} e_{R}\right) \\ & g_{2 L}\left(\overline{d_{R}^{c}} \gamma^{\mu} \nu_{L}\right), g_{2 R}\left(\overline{u_{L}^{c}} \gamma^{\mu} e_{R}\right) \end{aligned}$ |
| $\tilde{V}_{2 \mu}$ | $\begin{aligned} & \tilde{V}_{2 \mu}^{+} \\ & \tilde{V}_{2 \mu}^{-} \\ & \hline \end{aligned}$ | 1 | -2 | $\overline{3}$ | $\begin{aligned} & +\frac{1}{2} \\ & -\frac{1}{2} \end{aligned}$ | $-\frac{1}{6}$ | $\begin{array}{r} \frac{1}{3} \\ -\frac{2}{3} \\ \hline \end{array}$ | $\begin{aligned} & \tilde{g}_{2 L}\left(\overline{u_{R}^{c}} \gamma^{\mu} e_{L}\right) \\ & \tilde{g}_{2 L}\left(\overline{u_{R}^{c}} \gamma^{\mu} \nu_{L}\right) \\ & \hline \end{aligned}$ |
| $\bar{S}_{3}$ | $\begin{gathered} S_{3}^{+} \\ S_{3}^{0} \\ S_{3}^{-} \\ \hline \end{gathered}$ | 0 | -2 | $\overline{3}$ | $\begin{array}{r} \hline+1 \\ 0 \\ -1 \end{array}$ | $\frac{1}{3}$ | $\begin{array}{r} \frac{4}{3} \\ \frac{1}{3} \\ -\frac{2}{3} \\ \hline \end{array}$ | $\begin{gathered} -\sqrt{2} g_{3 L}\left(\overline{d_{L}^{c}} e_{L}\right) \\ -g_{3 L}\left(\overline{u_{L}^{c}} e_{L}+\overline{d_{L}^{c}} \nu_{L}\right) \\ \sqrt{2} g_{3 L}\left(\overline{u_{L}^{c}} \nu_{L}\right) \\ \hline \end{gathered}$ |
| $S_{2}$ | $S_{2}^{+}$ $S_{2}^{-}$ $\tilde{S}^{-}$ | 0 | 0 | 3 | $\begin{aligned} & \hline+\frac{1}{2} \\ & -\frac{1}{2} \end{aligned}$ | $\frac{7}{6}$ | $\frac{5}{3}$ <br> $\frac{2}{3}$ | $\begin{gathered} \hline \hline h_{2 L}\left(\overline{u_{R}} e_{L}\right), h_{2 R}\left(\overline{u_{L}} e_{R}\right) \\ h_{2 L}\left(\overline{u_{R}} \nu_{L}\right),-h_{2 R}\left(\overline{d_{L}} e_{R}\right) \end{gathered}$ |
| $\tilde{S}_{2}$ | $\begin{aligned} & \tilde{S}_{2}^{+} \\ & \tilde{S}_{2}^{-} \end{aligned}$ | 0 | 0 | 3 | $\begin{aligned} & +\frac{1}{2} \\ & -\frac{1}{2} \end{aligned}$ | $\frac{1}{6}$ | $\begin{array}{r} \frac{2}{3} \\ -\frac{1}{3} \\ \hline \end{array}$ | $\begin{aligned} & \tilde{h}_{2 L}\left(\overline{d_{R}} e_{L}\right) \\ & \tilde{h}_{2 L}\left(\overline{d_{R}} \nu_{L}\right) \end{aligned}$ |
| $V_{1 \mu}$ | $V_{1 \mu}^{0}$ | 1 | 0 | 3 | 0 | $\frac{2}{3}$ | $\frac{2}{3}$ | $h_{1 L}\left(\overline{u_{L}} \gamma^{\mu} \nu_{L}+\overline{d_{L}} \gamma^{\mu} e_{L}\right), h_{1 R}\left(\overline{d_{R}} \gamma^{\mu} e_{R}\right)$ |
| $\vec{V}_{1 \mu}$ | $\stackrel{V}{1 \mu}_{0}^{0}$ | 1 | 0 | 3 | 0 | $\frac{5}{3}$ | $\overline{3}$ | $\hat{h}_{1 R}\left(\overline{u_{R}} \gamma^{\mu} e_{R}\right)$ |
| $\vec{V}_{3 \mu}$ | $\begin{gathered} \hline V_{3 \mu}^{+} \\ V_{3 \mu}^{0} \\ V_{3 \mu}^{-} \\ \hline \hline \end{gathered}$ | 1 | 0 | 3 | +1 0 -1 | $\frac{2}{3}$ | $\begin{array}{r} \frac{5}{3} \\ \frac{2}{3} \\ -\frac{1}{3} \\ \hline \hline \end{array}$ | $\begin{gathered} \sqrt{2} h_{3 L}\left(\overline{u_{L}} \gamma^{\mu} e_{L}\right) \\ h_{3 L}\left(\overline{u_{L}} \gamma^{\mu} \nu_{L}-\overline{d_{L}} \gamma^{\mu} e_{L}\right) \\ \sqrt{2} h_{3 L}\left(\overline{d_{L}} \gamma^{\mu} \nu_{L}\right) \\ \hline \hline \end{gathered}$ |

TABLE IX: Quantum numbers of scalar and vector leptoquarks with $S U(3)_{C} \times S U(2)_{L} \times U(1)_{Y}$ invariant couplings to quarklepton pairs $\left(Q_{\mathrm{em}}=I_{3}+Y\right)[12$.

| $L Q$ | $C_{L}$ | $C_{R}$ | $\left\|\lambda_{L Q}\right\|^{2}$ | NuSOnG 95\% bound | $95 \%$ bound from $R_{\pi}$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $S_{1}$ | $s^{2}\left(\frac{4}{3}-\frac{10}{9} s^{2}\right)$ | $-\frac{10}{9} s^{4}$ | $\left\|g_{1 L}^{12}\right\|^{2}$ | 0.0036 | 0.0037 |
| $\vec{S}_{3}$ | $+\frac{10}{9} s^{4}$ | $+\frac{10}{9} s^{4}$ | $\left\|g_{3 L}^{12}\right\|^{2}$ | 0.010 | 0.0008 |
| $S_{2}$ | 0 | $-\frac{8}{3} s^{2}$ | $\left\|h_{2 L}^{12}\right\|^{2}$ | 0.0013 | N/A |
| $\tilde{S}_{2}$ | 0 | $+\frac{4}{3} s^{2}$ | $\left\|\tilde{h}_{2 L}^{12}\right\|^{2}$ | 0.0026 | N/A |
| $V_{1}$ | $s^{2}\left(\frac{4}{3}-\frac{20}{9} s^{2}\right)$ | $-\frac{20}{9} s^{4}$ | $\left\|h_{1 L}^{12}\right\|^{2}$ | 0.0040 | 0.0018 |
| $\vec{V}_{3}$ | $-4 s^{2}\left(1-\frac{5}{9} s^{2}\right)$ | $+\frac{20}{9} s^{4}$ | $\left\|h_{3 L}^{12}\right\|^{2}$ | 0.0011 | 0.0004 |
| $V_{2}$ | 0 | $-\frac{4}{3} s^{2}$ | $\left\|g_{2 L}^{12}\right\|^{2}$ | 0.0026 | N/A |
| $\vec{V}_{2}$ | 0 | $+\frac{8}{3} s^{2}$ | $\left\|\tilde{g}_{2 L}^{12}\right\|^{2}$ | 0.0013 | N/A |

TABLE X: Potential and existing $95 \%$ bounds on the leptoquark couplings squared when the leptoquark masses are set to 100 GeV . To obtain the limits for different leptoquark masses, multiply by $\left(M_{L Q} / 100 \mathrm{GeV}\right)^{2}$. Existing bounds on the $S_{1}, \vec{S}_{3}$, $V_{1}$, and $\vec{V}_{3}$ couplings from $R_{\pi}=\operatorname{Br}(\pi \rightarrow e \nu) / \operatorname{Br}(\pi \rightarrow \mu \nu)$ are also shown.

First, extend the Standard Model to include a nondegenerate $S U(2)_{L}$ triplet leptoquark $\left(\vec{S}_{3}\right.$ or $\vec{V}_{3}$ in the notation of [66], with masses in the $0.5-1.5 \mathrm{TeV}$ range. At the LHC these leptoquarks will be produced primarily in pairs through gluon fusion, and each leptoquark will decay to a lepton and a jet [72]. The peak in the lepton-jet invariant mass distribution will be easily detected over background. This will provide the leptoquark masses but yield little information about their couplings to fermions. The leptoquarks will also shift the neutrinonucleon effective coupling $g_{L}^{2}$ in a way that depends sensitively on both the leptoquark couplings and masses. Such a leptoquark-induced shift could provide an explanation for the NuTeV anomaly 61, 67, 73]. In this scenario, NuSOnG would find that isospin and the strange sea can be constrained to the point that they do not provide an explanation for the NuTeV anomaly, thus the NuTeV anomaly is the result of new physics. The NuSOnG PW
measurement of $\sin 2 \theta_{W}$ will agree with $\mathrm{NuTeV} ; g_{R}^{2}$ and the $\nu e$ and $\bar{\nu} e$ elastic scattering measurements will agree with LEP. Fig. 15 illustrates this example. NuSOnG's measurement of $g_{L}^{2}$ would provide a sensitive measurement of the leptoquark couplings when combined with the LHC mass measurements as inputs.

A second example is the existence of a fourth generation family. A fourth family with non-degenerate masses (i.e. isospin violating) is allowed within the LEP/SLD constraints 74. As a model, we choose a fourth family with mass splitting on the order of $\sim 75 \mathrm{GeV}$ and a 300 GeV Higgs. This is consistent with LEP at $1 \sigma$ and perfectly consistent with $M_{W}$, describing the point $(0.2,0.19)$ on the $S T$ plot. In this scenario, LHC will measure the Higgs mass from the highly enhanced $H \rightarrow Z Z$ decay. An array of exotic decays which will be difficult to fully reconstruct, such as production of 6 W 's and 2 b 's, will be observed at low rates. In this scenario, isospin


FIG. 14: Shifts in $g_{L}^{2}$ and $g_{R}^{2}$ due to leptoquarks. Horizontal lines indicate the projected $1 \sigma$ limits of NuSOnG.


FIG. 15: NuSOnG expectation in the case of a Tev-scale triplet leptoquark. For clarity, this plot and the two following cases, show the expectation from only the two highest precision measurements from NuSOnG: $g_{L}^{2}$ and $\nu$ ES.
violation explains the NuTeV anomaly, thus the NuTeV PW and the NuSOnG PW measurements agree with the $\nu$ eES measurements. These three precision neutrino results, all with "LEP-size" errors, can be combined and will intersect the one-sigma edge of the LEP measurements. Fig. 16 illustrates this example. From this, the source, a fourth generation with isospin violation, can be


FIG. 16: NuSOnG expectation if the NuTeV anomaly is due to isospin violation and there is a heavy 4th generation with isospin violation.


FIG. 17: If LHC sees a Standard Model Higgs and no evidence of new physics, NuSOnG may reveal new physics in the neutrino sector.
demonstrated.
Lastly, while it seems unlikely, it is possible that LHC will observe a Standard Model Higgs and no signatures of new physics. If this is the case, it is still possible for NuSOnG to add valuable clues to new physics. This is because the experiment is uniquely sensitive to the neutrino sector. If a situation such as is illustrated on Fig. 17 arose, the only explanation would be new physics unique to neutrino interactions.

## VI. SUMMARY AND CONCLUSIONS

NuSOnG is an experiment which can search for new physics from keV through TeV energy scales, as well as make interesting QCD measurements. This article has focussed mainly on the Terascale physics which can be accessed through this new high energy, high statistics
neutrino scattering experiment. The case has been made that this new neutrino experiment would be a valuable addition to the presently planned suite of experiments with Terascale reach.

The NuSOnG experiment design draws on the heritage of the CHARM II and CCFR/NuTeV experiments. A high energy, flavor-pure neutrino flux is produced using 800 GeV protons from the Tevatron. The detector consists of four modules, each composed of a finelysegmented glass-target $\left(\mathrm{SiO}_{2}\right)$ calorimeter followed by a muon spectrometer. In its five-year data acquisition period, this experiment will record almost one hundred thousand neutrino-electron elastic scatters and hundreds of millions of deep inelastic scattering events, exceeding the current world data sample by more than an order of magnitude. This experiment can address concerns related to model systematics of electroweak measurements in neutrino-quark scattering by direct constraints using $i n$-situ structure function measurements.

NuSOnG will be unique among present and planned experiments for its ability to probe neutrino couplings to Beyond Standard Model physics. This experiment offers four distinct and complementary probes of $S$ and $T$. Two are of high precision with the proposed run-plan, and the precision of the other two would be improved by a follow-up five-year antineutrino run. Neutrino-lepton non-standard interactions can be probed with an order of magnitude improvement in the measured effective couplings. Neutrino-quark non-standard interactions can be probed by an improvement in the measured neutrinoquark effective couplings of a factor of two or better. The
experiment is sensitive to new physics up to energy scales $\sim 5 \mathrm{TeV}$ at $95 \%$ CL. The measurements are sensitive to universality of the couplings and an improvement in the $e$-family of $30 \%$ and $\mu$-family of $75 \%$ will allow for probes of neutrissimos. As a unique contribution, NuSOnG measures $g_{R} / g_{L}$, which is not accessible by other near-future experiments. This article described NuSOnG's physics contribution under several specific models. These included models of $Z^{\prime}$ s, extended Higgs models, leptoquark models and $R$-parity violating SUSY models. We also considered how, once data are taken at LHC and NuSOnG, the underlying physics can be extracted. The opportunity for direct searches related to these indirect electroweak searches was also described. The conclusion of our analysis is that a new neutrino experiment, such as NuSOnG, would substantially enhance the presently planned Terascale program.

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# Expression of Interest for Neutrinos Scattering on Glass: NuSOnG 

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#### Abstract

We propose a 3500 ton ( 3000 ton fiducial volume) $\mathrm{SiO}_{2}$ neutrino detector with sampling calorimetry, charged particle tracking, and muon spectrometers to run in a Tevatron Fixed Target Program. Improvements to the Fermilab accelerator complex should allow substantial increases in the neutrino flux over the previous NuTeV quad triplet beamline. With $4 \times 10^{19}$ protons on target/year, a 5 year run would achieve event statistics more than 100 times higher than NuTeV . With 100 times the statistics of previous high energy neutrino experiments, the purely weak processes $\nu_{\mu}+e^{-} \rightarrow$ $\nu_{\mu}+e^{-}$and $\nu_{\mu}+e^{-} \rightarrow \nu_{e}+\mu^{-}$(inverse muon decay) can be measured with high accuracy for the first time. The inverse muon decay process is independent of strong interaction effects and can be used to significantly improve the flux normalization for all other processes. The high neutrino and antineutrino fluxes also make new searches for lepton flavor violation and neutral heavy leptons possible. In this document, we give a first look at the physics opportunities, detector and beam design, and calibration procedures.


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## 1 Introduction

The Neutrino Scattering on Glass (NuSOnG) experiment will consist of four detector modules, each composed of a finely segmented calorimeter followed by a muon spectrometer. The detector will be illuminated by a neutrino or antineutrino beam from the Tevatron. In its five-year data acquisition period, NuSOnG will make precise measurements of three types of neutrino scattering and will accumulate the world's largest sample of electron-neutrino scatters. These data will provide unique opportunities to discover physics beyond the Standard Model (including, inter alia, lepton flavor violation and new particles) as well as determine structure functions over a wide range of $x$ and $Q^{2}$. The breadth of anticipated measurements makes NuSOnG a program rather than an experiment; the design heritage ensures that the approach is low-risk and cost-effective.

This Expression of Interest arises from our view that an experiment probing the high energy interactions of neutrinos is a necessary complement to the LHC and an important lead-in to the ILC. In the next few years, the LHC will reveal the nature of electroweak symmetry breaking; the Higgs mass will cease being a prediction of the electroweak theory and will become an input to the theory. Without the Higgs mass as a fit parameter, precision electroweak data, including neutrino scattering data, will be much more powerful as a tool for constraining that physics beyond the Standard Model which directly influences the electroweak sector. More important still, precision neutrino scattering will probe areas of phenomenology that may be inaccessible to the LHC and ILC. NuSOnG is not a precision test of the Standard Model; NuSOnG is a discovery experiment aimed at the terrain not covered by the collider experiments.

This Expression of Interest presents the physics case and initial design for NuSOnG. The detector draws on the heritage of FMMF, CDHS, CHARM and CCFR/NuTeV. The design uses an $\mathrm{SiO}_{2}$ target in one-quarter radiation length panels interleaved with active detector elements (proportional tubes and/or scintillator). This will provide the very high segmentation needed to ensure good separation between different classes of events. We will develop these ideas in the coming months and submit a proposal to the Fermilab Directorate.

Our report is organized as follows: the physics opportunities follow in Section 2, Section 3 describes the flux and expected event rates; and Section 4 describes our preliminary design for the NuSOnG beam and apparatus. We summarize in Section 5 .

## 2 Physics Opportunities

The physics opportunities of the experiment arise from NuSOnG's uniquely high statistics: $>20 \mathrm{k}$ neutrino-electron scatters and $>100 \mathrm{M}$ neutrino-quark scatters. Roughly equal statistics will be obtained from antineutrino scattering. More information on the event rates for various processes is given in Sec. 3. These rates present a wide range of physics opportunities including precision electroweak measurements, direct searches for new physics, and parton distribution studies.

### 2.1 Electroweak Precision Measurements

NuSOnG's considerable discovery potential derives from its ability to do precision electroweak tests through two independent channels: electron scattering and quark scattering. These measurements probe for new particles and new neutrino properties beyond the present Standard Model. As examples, NuSOnG will be sensitive to extra $Z$ bosons with masses beyond the 1 TeV scale (depending on the model), and to compositeness scales above 5 TeV . Thus the energy scales explored by this experiment overlap the LHC, and we present the discovery potential for the new physics we will explore within this context. This experiment also directly addresses questions raised by the "NuTeV anomaly," an electroweak precision measurement in disagreement with the Standard Model.

### 2.1.1 Electroweak Measurements in Neutrino Scattering

NuSOnG is sensitive to new physics through neutral current (NC) scattering. The exchange of the $Z$ boson between the neutrino $\nu$ and fermion $f$ leads to the effective interaction:

$$
\left.\left.\left.\left.\begin{array}{rl}
\mathcal{L}= & -\sqrt{2} G_{F}[
\end{array}\right] \bar{\nu} \gamma_{\mu}\left(g_{V}^{\nu}-g_{A}^{\nu} \gamma_{5}\right) \nu\right]\left[\bar{f} \gamma^{\mu}\left(g_{V}^{f}-g_{A}^{f} \gamma_{5}\right) f\right]\right] \text { - } \sqrt{2} G_{F}\left[g_{L}^{\nu} \bar{\nu} \gamma_{\mu}\left(1-\gamma_{5}\right) \nu+g_{R}^{\nu} \bar{\nu} \gamma_{\mu}\left(1+\gamma_{5}\right) \nu\right]\right] .
$$

where the Standard Model values of the couplings are:

$$
\begin{align*}
g_{L}^{\nu} & =\sqrt{\rho}\left(+\frac{1}{2}\right) \\
g_{R}^{\nu} & =0 \\
g_{L}^{f} & =\sqrt{\rho}\left(I_{3}^{f}-Q^{f} \sin ^{2} \theta_{W}\right), \\
g_{R}^{f} & =\sqrt{\rho}\left(-Q^{f} \sin ^{2} \theta_{W}\right), \tag{2}
\end{align*}
$$

or equivalently,

$$
\begin{aligned}
& g_{V}^{\nu}=g_{L}^{\nu}+g_{R}^{\nu}=\sqrt{\rho}\left(+\frac{1}{2}\right) \\
& g_{A}^{\nu}=g_{L}^{\nu}-g_{R}^{\nu}=\sqrt{\rho}\left(+\frac{1}{2}\right)
\end{aligned}
$$

$$
\begin{align*}
& g_{V}^{f}=g_{L}^{f}+g_{R}^{f}=\sqrt{\rho}\left(I_{3}^{f}-2 Q^{f} \sin ^{2} \theta_{W}\right), \\
& g_{A}^{f}=g_{L}^{f}-g_{R}^{f}=\sqrt{\rho}\left(I_{3}^{f}\right) . \tag{3}
\end{align*}
$$

Here, $I_{3}^{f}$ and $Q^{f}$ are the weak isospin and electromagnetic charge of fermion $f$, respectively. In these formulae, $\rho$ is the relative coupling strength of the neutral to charged current interactions ( $\rho=1$ at tree level in the Standard Model). The weak mixing parameter, $\sin ^{2} \theta_{W}$, is related (at tree level) to to $G_{F}, M_{Z}$ and $\alpha$ by

$$
\begin{equation*}
\sin ^{2} 2 \theta_{W}=\frac{4 \pi \alpha}{\sqrt{2} G_{F} M_{Z}^{2}} \tag{4}
\end{equation*}
$$

NuSOnG is unique in its ability to test the NC couplings by studying scattering of neutrinos from both electrons and quarks. A deviation from the Standard Model predictions in both the electron and quark measurements will present a compelling case for new physics.

## Neutrino Electron Scattering

The differential cross section for muon neutrino and antineutrino scattering from electrons, defined using the coupling constants described above, is:

$$
\begin{align*}
d \sigma=\frac{2 G_{F}^{2} m_{e} E_{\nu}}{\pi} & {\left[\left(g_{L}^{\nu} g_{V}^{e} \pm g_{L}^{\nu} g_{A}^{e}\right)^{2} \frac{d T}{E_{\nu}}\right.} \\
& +\left(g_{L}^{\nu} g_{V}^{e} \mp g_{L}^{\nu} g_{A}^{e}\right)^{2}\left(1-\frac{T}{E_{\nu}}\right)^{2} \frac{d T}{E_{\nu}} \\
& \left.-\left\{\left(g_{L}^{\nu} g_{V}^{e}\right)^{2}-\left(g_{L}^{\nu} g_{A}^{e}\right)^{2}\right\} \frac{m_{e} T}{E_{\nu}^{2}} \frac{d T}{E_{\nu}}\right] \tag{5}
\end{align*}
$$

The upper and lower signs corresponding to the neutrino and anti-neutrino cases, respectively. In this equation, $E_{\nu}$ is the incident $\nu_{\mu}$ energy and $T$ is the electron recoil kinetic energy.

More often in the literature, the cross section is defined in terms of the parameters $\left(g_{V}^{\nu e}, g_{A}^{\nu e}\right)$, which are defined as

$$
\begin{align*}
g_{V}^{\nu e} & \equiv\left(2 g_{L}^{\nu} g_{V}^{e}\right)=\rho\left(-\frac{1}{2}+2 \sin ^{2} \theta_{W}\right) \\
g_{A}^{\nu e} & \equiv\left(2 g_{L}^{\nu} g_{A}^{e}\right)=\rho\left(-\frac{1}{2}\right) \tag{6}
\end{align*}
$$

In terms of these parameters, we can write:

$$
\begin{align*}
d \sigma=\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi} & {\left[\left(g_{V}^{\nu e} \pm g_{A}^{\nu e}\right)^{2} \frac{d T}{E_{\nu}}+\left(g_{V}^{\nu e} \mp g_{A}^{\nu e}\right)^{2}\left(1-\frac{T}{E_{\nu}}\right)^{2} \frac{d T}{E_{\nu}}\right.} \\
& \left.-\left\{\left(g_{V}^{\nu e}\right)^{2}-\left(g_{A}^{\nu e}\right)^{2}\right\} \frac{m_{e} T}{E_{\nu}^{2}} \frac{d T}{E_{\nu}}\right] \tag{7}
\end{align*}
$$

When $m_{e} \ll E_{\nu}$, the third terms in these expressions can be neglected. If we introduce the variable $y=T / E_{\nu}$, then

$$
\begin{equation*}
\frac{d \sigma}{d y}=\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi}\left[\left(g_{V}^{\nu e}+g_{A}^{\nu e}\right)^{2}+\left(g_{V}^{\nu e}-g_{A}^{\nu e}\right)^{2}(1-y)^{2}\right] \tag{8}
\end{equation*}
$$

Integrating over the region $0 \leq y \leq 1$, we obtain the total cross sections which are

$$
\begin{equation*}
\sigma=\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi}\left[\left(g_{V}^{\nu e} \pm g_{A}^{\nu e}\right)^{2}+\frac{1}{3}\left(g_{V}^{\nu e} \mp g_{A}^{\nu e}\right)^{2}\right] \tag{9}
\end{equation*}
$$

Note that

$$
\begin{align*}
& \left(g_{V}^{\nu e}+g_{A}^{\nu e}\right)^{2}=\rho^{2}\left(-1+4 \sin ^{2} \theta_{W}\right)^{2}=\rho^{2}\left(1-2 \sin ^{2} \theta_{W}+4 \sin ^{4} \theta_{W}\right) \\
& \left(g_{V}^{\nu e}-g_{A}^{\nu e}\right)^{2}=\rho^{2}\left(2 \sin ^{2} \theta_{W}\right)^{2}=\rho^{2}\left(4 \sin ^{4} \theta_{W}\right) \tag{10}
\end{align*}
$$

Therefore,

$$
\begin{align*}
\sigma\left(\nu_{\mu} e\right) & =\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi} \rho^{2}\left[1-4 \sin ^{2} \theta_{W}+\frac{16}{3} \sin ^{4} \theta_{W}\right] \\
\sigma\left(\bar{\nu}_{\mu} e\right) & =\frac{G_{F}^{2} m_{e} E_{\nu}}{2 \pi} \frac{\rho^{2}}{3}\left[1-4 \sin ^{2} \theta_{W}+16 \sin ^{4} \theta_{W}\right] \tag{11}
\end{align*}
$$

The ratio of the integrated cross sections for neutrino to antineutrino electron scattering is

$$
\begin{equation*}
R_{e}=\frac{\sigma\left(\nu_{\mu L} e\right)}{\sigma\left(\bar{\nu}_{\mu L} e\right)}=3 \frac{1-4 \sin ^{2} \theta_{W}+\frac{16}{3} \sin ^{4} \theta_{W}}{1-4 \sin ^{2} \theta_{W}+16 \sin ^{4} \theta_{W}} \tag{12}
\end{equation*}
$$

Many systematics, including flux errors, cancel in this ratio, as does the $\rho$ dependence. Fig. 1(top) shows the results for $\sin ^{2} \theta_{W}$ from many past experiments.

NuSOnG will make independent measurements of the electroweak parameters for both $\nu_{\mu}$ and $\bar{\nu}_{\mu}$-electron scattering. We can achieve this via ratios or by direct extraction of the cross section. In the case of $\nu_{\mu}$-electron scattering, we will use the ratio of the number of events in neutrino-electron elastic scattering to inverse muon decay:

$$
\begin{equation*}
\frac{N\left(\nu_{\mu} e^{-} \rightarrow \nu_{\mu} e^{-}\right)}{N\left(\nu_{\mu} e^{-} \rightarrow \mu^{-} \nu_{e}\right)}=\frac{\sigma_{N C}^{\nu e} \times \Phi^{\nu}}{\sigma^{I M D} \times \Phi^{\nu}} \tag{13}
\end{equation*}
$$

Because the cross section for IMD events is well determined by the standard model, this ratio should have low errors and will isolate the EW parameters from NC scattering. In the case of $\bar{\nu}_{\mu}$ running, the ratio is more complex because there is no equivalent process to inverse muon decay (since there are no positrons in the detector). In this case, we use the fact that, for low exchange energy in Deep Inelastic Scattering, the cross sections in neutrino and antineutrino scattering approach the same constant, $A$, as is explained in Sec. 3.3.2. Thus, for Deep Inelastic events with low energy transfer and hence low hadronic energy $\left(5 \lesssim E_{h a d} \lesssim 10 \mathrm{GeV}\right), N_{\nu D I S}^{l o w} E_{h a d}=\Phi^{\nu} A$ and $N_{\bar{\nu} D I S}^{l o w}{ }_{h} a d=\Phi^{\bar{\nu}} A$. The result is that we can extract the electroweak parameters to high precision using the ratio:

$$
\begin{equation*}
\frac{N_{\nu D I S}^{l o w} E_{\text {had }}}{N_{\bar{\nu} D I S}^{\text {low } E_{\text {had }}}} \times \frac{N\left(\bar{\nu}_{\mu} e^{-} \rightarrow \bar{\nu}_{\mu} e^{-}\right)}{N\left(\nu_{\mu} e^{-} \rightarrow \mu^{-} \nu_{e}\right)}=\frac{\Phi^{\nu}}{\Phi^{\bar{\nu}}} \times \frac{\sigma_{N C}^{\bar{\nu} e} \times \Phi^{\bar{\nu}}}{\sigma^{I M D} \times \Phi^{\nu}} \tag{14}
\end{equation*}
$$

The first ratio cancels the DIS cross section, leaving the energy-integrated $\nu$ to $\bar{\nu}$ flux ratio. The IMD events in the denomenator of the second term cancel the integrated $\nu$ flux. The NC elastic events cancel the integrated $\bar{\nu}$ flux. Alternatively, because we will have accurate knowledge of the flux as a function of the energy (see Sec. 3.3) we could directly measure the cross sections.


Figure 1: Measurements of $\sin ^{2} \theta_{W}$ from past experiments. Top: neutrino-electron elastic scattering experiments. Bottom: neutrino DIS experiments. All DIS results are adjusted to the same charm mass (relevant for experiments not using P-W method). The Standard Model value, indicated by the line, is 0.2227 .

An important point is that the two independent measurements, one in neutrino and the other in antineutrino mode, will in turn allow independent extraction of $g_{A}^{\nu e}$ and $g_{V}^{\nu e}$. The previous best measurement from $\nu_{\mu}$ and $\bar{\nu}_{\mu}$ cross-section measurements is from CHARM II, which used $2677 \pm 82$ events in neutrino mode and $2752 \pm 88$ events in antineutrino mode [1] to find

$$
\begin{gather*}
g_{V}^{\nu e}=-0.035 \pm 0.012(\text { stat }) \pm 0.012(\mathrm{sys})  \tag{15}\\
g_{A}^{\nu e}=-0.503 \pm 0.006(\text { stat }) \pm 0.016(\mathrm{sys}) \tag{16}
\end{gather*}
$$

This can be compared to electroweak measurements from LEP provide a very precise prediction of these parameters [2]:

$$
\begin{align*}
g_{V}^{\nu e} & =-0.0397 \pm 0.0003  \tag{17}\\
g_{A}^{\nu e} & =-0.5065 \pm 0.0001 . \tag{18}
\end{align*}
$$

The CHARM II results are in agreement with LEP, but with large errors. Errors on the neutrino measurement must be substantially reduced in order to meaningfully probe for physics beyond the Standard Model. The goal of NuSOnG is to measure the neutrino-electron and antineutrino-electron cross sections to $0.7 \%$.

### 2.1.1.1 Neutrino Quark Scattering

Substantially higher precision has been obtained using neutrino-quark scattering, which compares neutral-current (NC) to charged-current (CC) scattering to extract $\sin ^{2} \theta_{W}$. However, these experiments are subject to issues of modeling in the quark sector. Fig. 1(bottom) reviews the history of these measurements.

The lowest systematic errors come from implementing a "Paschos-Wolfenstein style" [3] analysis, which would be the technique used by NuSOnG. This requires separated $\nu$ and $\bar{\nu}$ beams, for which the following ratios could be formed:

$$
\begin{align*}
R^{\nu} & =\frac{\sigma_{N C}^{\nu}}{\sigma_{C C}^{\nu}}  \tag{19}\\
R^{\bar{\nu}} & =\frac{\sigma_{N C}^{\bar{\nu}}}{\sigma_{C C}^{\bar{\nu}}} \tag{20}
\end{align*}
$$

Paschos and Wolfenstein [3] recast these as:

$$
\begin{equation*}
R^{-}=\frac{\sigma_{N C}^{\nu}-\sigma_{N C}^{\bar{\nu}}}{\sigma_{C C}^{\nu}-\sigma_{C C}^{\bar{\nu}}}=\frac{R^{\nu}-r R^{\bar{\nu}}}{1-r} \tag{22}
\end{equation*}
$$

where $r=\sigma_{C C}^{\bar{\nu}} / \sigma_{C C}^{\nu}$. In $R^{-}$many systematics cancel to first order, including the effects of the quark and antiquark seas for $u, d, s$, and $c$. Charm production only enters through $d_{\text {valence }}$ (which is Cabbibo suppressed) and at high $x$; thus the error from the charm mass is greatly reduced. The cross section ratios can be written in terms of the effective neutrino-quark coupling parameters $g_{L}^{2}$ and $g_{R}^{2}$ as

$$
\begin{align*}
R^{\nu} & =g_{L}^{2}+r g_{R}^{2}  \tag{23}\\
R^{\bar{\nu}} & =g_{L}^{2}+\frac{1}{r} g_{R}^{2}  \tag{24}\\
R^{-} & =g_{L}^{2}-g_{R}^{2}=\rho^{2}\left(\frac{1}{2}-\sin ^{2} \theta_{W}\right) \tag{25}
\end{align*}
$$

| Source | Error | Reduction in NuSOnG |
| :---: | :---: | :---: |
| Statistics | 0.00135 | 100 times the statistics |
| $\nu_{e}, \bar{\nu}_{e}$ flux prediction | 0.00039 | see Sec. 3.3 .6 |
| Interaction vertex position | 0.00030 | Better detector segmentation and <br> more sophisticated shower identification. |
| Shower length model | 0.00027 | Better segmentation and <br> more sophisticated shower identification. |
| Counter efficiency and noise | 0.00023 | Better, Minos-style counter design |
| Energy Measurement | 0.00018 | Likely to be at a similar level. |
| Charm production, strange sea | 0.00047 | See Sec. 2.4 .4 |
| $R_{L}$ | 0.00032 | Likely to be at a similar level. |
| $\sigma^{\bar{\nu}} / \sigma^{\nu}$ | 0.00022 | See Sec. 2.4 .5 |
| Higher Twist | 0.00014 | Likely to be at a similar level. |
| Radiative Corrections | 0.00011 | Likely to be at a similar level. |
| Charm Sea | 0.00010 | Under study |
| Non-isoscalar target | 0.00005 | Glass is isoscalar |

Table 1: Source and value of NuTeV error on $\sin ^{2} \theta_{W}$, and reason why the error will be reduced in the PW-style analysis of NuSOnG.
in which

$$
\begin{align*}
g_{L}^{2} & =\left(2 g_{L}^{\nu} g_{L}^{u}\right)^{2}+\left(2 g_{L}^{\nu} g_{L}^{d}\right)^{2}=\rho^{2}\left(\frac{1}{2}-\sin ^{2} \theta_{W}+\frac{5}{9} \sin ^{4} \theta_{W}\right)  \tag{26}\\
g_{R}^{2} & =\left(2 g_{L}^{\nu} g_{R}^{u}\right)^{2}+\left(2 g_{L}^{\nu} g_{R}^{d}\right)^{2}=\rho^{2}\left(\frac{5}{9} \sin ^{4} \theta_{W}\right) \tag{27}
\end{align*}
$$

NuTeV fit for $R^{\nu}$ and $R^{\bar{\nu}}$ simultaneously to extract $\sin ^{2} \theta_{W}$, obtaining the value $\sin ^{2} \theta_{W}=0.2277 \pm 0.00162$. The goal of NuSOnG is to improve on this error by a factor of two. Table 1 lists the errors which NuTeV identified and indicates those for which NuSOnG expects improvement. Many of the largest experimental systematics of NuTeV came from the method of separating CC and NC events, which relied on length. NuSOnG will have a more sophisticated model for differentiating CC and NC events, using shower shape and identification of Michel-electron followers from low energy pion decays.

From Fig. 1, it is apparent that the NuTeV measurement is in agreement with past neutrino scattering results, although these have much larger errors. However, the NuTeV result is in disagreement with the global fits to the electroweak data which give a Standard Model value of $\sin ^{2} \theta_{W}=0.2227$ [4]. Expressed in terms of the couplings, NuTeV measures:

$$
\begin{gather*}
g_{L}^{2}=0.30005 \pm 0.00137  \tag{28}\\
g_{R}^{2}=0.03076 \pm 0.00110 \tag{29}
\end{gather*}
$$

which can be compared to the Standard Model values of $g_{L}^{2}=0.3042$ and $g_{R}^{2}=0.0301$, respectively. Sec. 2.2 (below) considers possible sources for this disagreement, both within and outside the Standard Model.

### 2.1.2 NuSOnG and New Physics

NuSOnG will provide important probes of physics beyond the Standard Model distinct from and complementary to those of the LHC. NuSOnG will seek indirect evidence for new physics by addressing anomalies in the precision electroweak data, and by providing unique information about neutrino coupling to the $Z$. In addition, precision measurements from NuSOnG will help to disentangle the complicated set of observations that will be present at the LHC and, in doing so, elucidate the mechanism of electroweak symmetry breaking. NuSOnG and the LHC provide distinct probes of new physics because new physics enters collider and neutrino scattering processes differently: neutrino physics measures different combinations of couplings to light quarks; neutrino scattering probes new physics at space-like momentum transfer (versus the time-like scattering at colliders); and systematics are very different between low and high energy experiments. Finally, NuSOnG will directly search for new particles and interactions in the lepton sector that might be missed by the LHC and must otherwise await discovery by the ILC.

### 2.1.2.1 New Physics Observed through Coupling to the $Z$

NuSOnG is unique among experiments in its ability to address the nature of the neutrino couplings to the $Z$ boson in the near future. In the Standard Model, the neutrino coupling to the $Z$ - and $W$-bosons is purely left-handed. Indeed, the fact that the neutrino coupling to the $W$-boson and an electron is purely left-handed is, experimentally, a well-established fact (evidence includes precision measurements of pion and muon decay, nuclear processes, etc.). By contrast, the nature of the neutrino coupling to the $Z$ boson is, experimentally, far from being precisely established [5].

The best measurement of the neutrino coupling to the $Z$-boson is provided by indirect measurements of the invisible $Z$-boson width at LEP. In units where the Standard Model neutrino- $Z$-boson couplings are $g_{L}^{\nu}=0.5, g_{R}^{\nu} \equiv 0$, the LEP measurement [6] translates into $\left(g_{L}^{\nu}\right)^{2}+\left(g_{R}^{\nu}\right)^{2}=0.2487 \pm 0.0010$. Note that this result places no meaningful bound on $g_{R}^{\nu}$.

Precise, model-independent information on $g_{L}^{\nu}$ can be obtained by combining $\nu_{\mu}+e$ scattering data from CHARM II and LEP and SLD data. Assuming model-independent couplings of the fermions to the $Z$-boson, $\nu_{\mu}+e$ scattering measures $g_{L}^{\nu}=2 \rho$, while LEP and SLD measure the left and right-handed couplings of the electron to the $Z$. The CHARM II result translates into $\left|g_{L}^{\nu}\right|=0.502 \pm 0.017$ [5], assuming that the charged-current weak interactions produce only left-handed neutrinos. In spite of the good precision of the CHARM II result (around 3.5\%), a combination of all available data allows $\left|g_{R}^{\nu} / g_{L}^{\nu}\right| \sim 0.4$ at the two $\sigma$ confidence level [5].

Significant improvement in our understanding of $g_{R}^{\nu}$ can only be obtained with more precise measurements of $\nu+e$ scattering, or with the advent of a new high intensity $e^{+} e^{-}$collider, such as the ILC. By combining ILC running at the $Z$-boson pole mass and at $\sqrt{s}=170 \mathrm{GeV},\left|g_{R}^{\nu} / g_{L}^{\nu}\right| \lesssim 0.3$ could be constrained at the two $\sigma$ level after analyzing $e^{+} e^{-} \rightarrow \gamma+$ missing energy events [5].

At NuSOnG, we estimate that $g_{L}^{\nu}$ can be measured at around the $0.86 \%$ level. This estimate is obtained by combining the statistical uncertainty $(20,000 \nu+e$ elastic scattering events) with an estimated $0.5 \%$ systematic uncertainty from the flux estimate. Fig. 2 (left) depicts an estimate of how precisely $g_{R}^{\nu}$ could be constrained if the Nu -


Figure 2: Precision with which the right-handed neutrino- $Z$-boson coupling can be determined by combining NuSOnG measurements of $g_{L}^{\nu}$ with the indirect determination of the invisible $Z$-boson width at LEP. In the left panel, we assume that the $\nu+e$ scattering measurement is consistent with the Standard Model prediction $g_{L}^{\nu}=0.5$, while in the right panel we assume that the $\nu+e$ scattering measurement is significantly lower, $g_{L}^{\nu}=0.485$, but still in agreement with the CHARM II measurement (at the one sigma level). Contours (black, red) are one and two sigma, respectively, while the star indicates the Standard Model expectation. See [5] for more details.

SOnG result, assumed to agree with the Standard Model prediction, is combined with the indirect LEP constraints. One can clearly see that this measurement $\left(\left|g_{R}^{\nu} / g_{L}^{\nu}\right| \lesssim 0.2\right.$ at the two sigma level) compares favorably with the ILC capabilities described above. If the NuSOnG result is incompatible with Standard Model expectations but still in agreement with the CHARM II experiment, a combined NuSOnG-LEP analysis should be able to establish that $g_{R}^{\nu} \neq 0$, as depicted in Fig. 2 (right).

### 2.1.2.2 New Physics Observed through Oblique Corrections

Precision neutrino scattering measurements made at NuSOnG can reveal new physics even when new particles are not created in the final state, through the effects of these particles in loops. For models of new physics in which the dominant loop corrections are vacuum polarization corrections to the gauge boson propagators ("oblique" corrections), the $S T$ parameterization introduced by Peskin and Takeuchi [7] provides a convenient framework in which to describe the effects of the new physics.

The $S T$ parameterization begins with a reference Standard Model, including reference values for the Higgs and top masses, and predictions for observables in this reference Standard Model. Differences between predicted and experimental values of the observables are then parameterized by and used to fit for $S$ and $T$, which can then be compared to predictions from new physics. The full set of precision electroweak data can then be used to constrain $S$ and $T$, as shown in Fig. 3. The $T$ parameter is


Figure 3: Three projected electroweak measurements from NuSOnG in S-T plane. LEP/SLD error ellipse is shown in red and the current $\mathrm{NuTeV} \nu-q$ measurement is shown as a light blue band. The ochre band shows NuSOnG $\bar{\nu}-e$, the dark blue band shows NuSOnG $\nu-q$ and the green shows NuSOnG $\nu-e$. The width of the bands correspond to $68 \%$ confidence level for statistics as described in the text. The NuSOnG measurements assume $(S, T)=(0,0)$.
sensitive to new physics that violates isospin and is zero for new physics that conserves isospin. Isospin-breaking new physics such as heavy non-degenerate fermion doublets or scalar multiplets would affect the $T$ parameter. The $S$ parameter is sensitive to isospin-conserving physics, such as heavy degenerate fermion doublets.

The status of electroweak measurements are shown in Fig. 3 [8]. The combined analysis of the LEP and SLD data by the LEP Electroweak Working Group (EWWG) $[9$ indicates an allowed region shown by the small oval, centered at $S=0.05 \pm 0.10$ and $T=0.07 \pm 0.11$. A different choice of reference Higgs or top mass changes Standard Model predictions for observables and thus shifts the center of the $S T$ plot [10]; setting the Higgs mass to 1000 GeV would shift the center of the oval to roughly $(S, T)=$ $(0.12,-0.36)$. Measurements of the $W$ mass, which are not shown, are also consistent with the LEP measurements. The highest precision neutrino result comes from $\nu q$ and $\bar{\nu} q$ scattering by the NuTeV experiment. This result clearly disagrees with the other
measurements, as discussed in Sec. 2.2.
The goal of NuSOnG is to make measurements which are competitive with or better than past electroweak measurements. These goals are indicated by the magenta ellipse and orange band on Fig. 3. The magenta ellipse shows the area in $S T$ space which can be probed if a $0.7 \%$ measurement of the $\nu$ and $\bar{\nu}$ NC electron-scattering cross sections is achieved. The orange band shows the improvement in the neutrino-quark, "Paschos-Wolfenstein"-style measurement which is expected from NuSOnG.

Disregarding the NuTeV offset for the moment, one can now ask: how will this plot look in the era of LHC and what will NuSOnG add? We consider this question in light of three scenarios:

1. a light Higgs (115-200 GeV)
2. a heavy Higgs ( $200-1000 \mathrm{GeV}$ )
3. no Higgs signal.

### 2.1.2.3 NuSOnG Impact for a Light Higgs (115-200 GeV) Scenario

A light Higgs is consistent with LEP/SLD and $W$ mass data. The fit to the electroweak data excluding NuTeV indicates a mass less than 144 GeV at $95 \%$ CL. This is also consistent with the current best direct-search limit which finds $m_{H}>114 \mathrm{GeV}[9]$. In the case of the lightest Higgs masses, where the cleanest signal may be in $H \rightarrow \gamma \gamma$, a clear observation above background will be experimentally difficult and may take some time.

Once the LHC measurement of the Higgs mass is made, the center of the $S T$ ellipse (Fig. 3) will be fixed at a point (modulo any remaining uncertainty in the top mass). Our experiment is especially interesting if the NuSOnG result disagrees with this LEP+SLD+LHC point. If the LHC measurement is high, i.e. $m_{H} \sim 200 \mathrm{GeV}$, the result would be marginally inconsistent with the $M_{W}$ analysis, which is $85_{-28}^{+39} \mathrm{GeV} 9$. In this case, comparison with the $\nu_{\mu}$ scattering results from NuSOnG could resolve the question of a discrepancy between these measurements.

If all other electroweak results are in good agreement, but disagree with NuSOnG, this would indicate new properties associated exclusively with the neutrino. An example would be decreased coupling of the neutrino to the $Z$ boson, where suppression of the coupling comes from intergenerational mixing of the light neutrino with a moderately heavy neutrino:

$$
\begin{equation*}
\nu_{\mu}=(\cos \alpha) \nu_{\text {light }}+(\sin \alpha) \nu_{\text {heavy }} . \tag{30}
\end{equation*}
$$

The $Z \nu_{\mu} \nu_{\mu}$ coupling is modified by $\cos ^{2} \alpha$ and the $W \mu \nu_{\mu}$ coupling is modified by $\cos \alpha$. This model, inspired by the NuTeV anomaly (see Sec. 2.2), would yield a measurement in NuSOnG with a low NC-to-CC ratio in both the case of electron and quark scattering.

These moderately heavy right-handed states, dubbed "neutrissimos" [12], could have masses as low as just above the current bound of the $Z$ mass. They may well be within the reach of the LHC and may appear as missing energy in events [12. Some models allow for neutrissimos as light as $\sim 100 \mathrm{GeV}$ [13]. The neutrissimos decay very quickly, but not always invisibly. For example, in the reaction $N \rightarrow \ell+W$, the $W$ may decay to either two jets or a neutrino-charged-lepton pair; only the latter case has missing energy. This may make recognition of the neutrissimo at LHC rather
difficult. In the case of $m_{H}<130 \mathrm{GeV}$, a dominant decay mode of the Higgs (along with $b \bar{b}$ ) could be into $\nu N$, where the neutrissimo subsequently decays. Reconstructing the Higgs in this case may be difficult at LHC; if neutrissimos exist, the result from NuSOnG may significantly improve our understanding of LHC results.

With a large tuning among the neutrino Yukawa couplings [13] neutrissimos could be the seesaw right-handed neutrinos. Relatively "large" mixing is marginally consistent with other constraints, including neutrinoless double-beta decay, which constrains $\left|U_{e 4}\right|^{2}$ to be less than a few $\times 10^{-5}$ for a 100 GeV right-handed neutrino, and rare pion and tau decays, which constrain $\left|U_{\mu 4}\right|^{2}$ to be less than, most conservatively, 0.004 and $\left|U_{\tau 4}\right|^{2}$ to be less than 0.006 . Other bounds come from $\mu \rightarrow e$ conversion in nuclei and other charged-lepton-flavor violation. A new experiment to search for $\mu \rightarrow e$ has been proposed at Fermilab [14] should also be sensitive to neutrissimos. The combination of NuSOnG and this experiment will be powerful in identifying the existence of these particles.

If the neutrissimo is a Majorana particle, it could be instrumental in elucidating the mechanism for leptogenesis. The present models of leptogenesis require very high mass scales for the neutral lepton, but theorists are pursuing ways to accommodate lower masses [15]. There also may be a wide mass spectrum for these particles, with one very heavy state required by standard leptogenesis models and others with masses in the range observable at LHC [16].

### 2.1.2.4 NuSOnG Contribution in a Heavy Higgs (200-1000 GeV) Scenario

While present electroweak data excluding NuTeV favor a light Higgs ( $\lesssim 200 \mathrm{GeV}$ ), as indicated in Fig. 3, the Higgs mass can extend up to about 1000 GeV without violating unitarity [17]. Thus, if LHC finds that the Higgs is between ~200 and 1000 GeV and the LEP+SLD ellipse has no major systematic error, then new physics must explain the discrepancy. Candidate models of new physics may well affect the neutrino scattering and $e^{+} e^{-}$scattering differently, so the high-precision neutrino scattering measurements from NuSOnG will provide an important piece of the puzzle if the Higgs mass found at LHC is genuinely inconsistent with LEP + SLD predictions.

Introduction of a fourth family would compensate for a modestly heavy ( $\sim 300$ GeV ) Higgs by shifting the LEP + SLD allowed region back up in $S$ and $T$ [18]. This family would need to exist above the bounds of direct searches, which is $\gtrsim 300 \mathrm{GeV}$. Mixing must be confined within the allowed bounds of the CKM matrix measurements [20]. A nice feature of this model is that a fourth-generation Majorana neutrino could play the role of dark matter. Depending on the underlying physics, evidence of a fourth family would be apparent in a shift of the NuSOnG result on the $S T$ plot. This could be especially important if the physics introducing the fourth family is from a mechanism like "Top See Saw" [21, which will not be observable at LHC. The impact of this particular model on neutrino scattering is not yet thoroughly explored, but could prove interesting [22].

A classic method for masking a heavy Higgs is to introduce heavy $Z$ bosons [23], which, as shown in ref. [10, tend to move the LEP-SLD ellipse upward in $T$, compensating for the heavy Higgs. Introduction of a $Z^{\prime}$ tends to increase NC rate in neutrino scattering and also to move the neutrino result upward on the $S T$ plot (although with a different dependence than the LEP-SLD result).

There are good theoretical reasons for considering the existence of additional neutral heavy gauge bosons. Extra $Z$ bosons appear in various GUT and string-motivated extensions to the Standard Model [24]. For example, the $E(6)$ breakdown to $S O(10) \times$ $U(1)_{\psi}$ results in the $Z_{\psi}$. The $S O(10)$ break down to $S U(5) \times U(1)_{\chi}$ yields the $Z_{\chi}$. Thus the new exchange boson could be: $Z^{\prime}=Z_{\chi} \cos \beta+Z_{\psi} \sin \beta$, where the mixing angle $\beta$ is an arbitrary parameter. Extra $Z$ bosons also appear in other beyond Standard Model theories, including extra dimensions with gauge fields in the bulk [25]; little Higgs theories [26], which use heavy $Z$ s to cancel divergences in the Higgs mass; and topcolor in which they drive electroweak symmetry breaking [27]. Heavy $Z \mathrm{~s}$ provide a mechanism for new SUSY theories to evade the LEP bound of $m_{H}=114 \mathrm{GeV}$ [28]. These models all produce new physics signatures at LHC. The precision measurement from NuSOnG can aid in differentiating models.

Models which introduce new physics to mask a heavy Higgs may seem contrived until one looks at the LEP+SLD data more closely. Up to this point we have considered the LEP+SLD measurements as a single result, however, many measurements enter this fit, and larger than expected inconsistencies between these measurements exist [29]. For example, there is a $3.2 \sigma$ discrepancy between the forward-backward $\left(A_{F B}\right)$ and leftright $\left(A_{L R}\right)$ asymmetry measurements. Excluding the $A_{F B}$ result, the LEP+SLD fit yields $m_{H}<115 \mathrm{GeV}$ at $95 \%$, with the best fit at 42 GeV - i.e. a range already excluded by direct searches, which require $m_{H}>114 \mathrm{GeV}$ at $95 \%$ CL.

There are several ways to interpret this deviation. It may simply be that there are systematics involved in the $A_{F B}$ measurement which have yet to be identified and which would bring this result into agreement with the others. In this case, we are in the dramatic situation of having already ruled out the Higgs. The scenario of no Higgs is considered in the next section. Alternatively, new physics is involved. This result is dominated by purely leptonic measurements. On the other hand, the fit to the hadronic asymmetries, dominated by $A_{F B}^{b}$ has two $\chi^{2}$ minima, at 450 and 3000 GeV . Thus, one may either introduce new physics which produces a $20 \%$ shift on $A_{F B}^{b}$ alone; or introduce new physics which would indicate apparently low values of $m_{H}$ in the lepton-based measurements, when actually the value is large. Within any of these scenarios, new precision results from NuSOnG will be valuable for understanding the underlying physics.

### 2.1.2.5 NuSOnG and the Case of No Higgs

Higgsless models do not employ the Higgs mechanism to render the Standard Model renormalizable [30]; instead they introduce some other scheme. The Higgs mechanism enforces unitarity in the scattering amplitudes of longitudinally polarized gauge bosons, $W_{L}^{ \pm}+Z_{L}^{o} \rightarrow W_{L}^{ \pm} Z_{L}^{o}$, for example. A requirement that the transition probability remains less than one gives the energy scale $\Lambda$ at which a new mechanism must come into play,

$$
\begin{equation*}
\Lambda \sim \frac{4 \pi M_{W}}{g} \sim 1.8 \mathrm{TeV} \tag{31}
\end{equation*}
$$

Higgsless theories generally contain new mass bosons $V_{i}$ with masses on the TeV scale that act to cancel the divergences in gauge boson scattering. Cancelling the amplitudes while respecting bounds from current electroweak couplings typically give small
couplings:

$$
\begin{equation*}
g_{W Z V}<\frac{g_{w w z} M_{Z}^{2}}{\sqrt{3} M_{1}^{ \pm} M_{W}}=0.04 \tag{32}
\end{equation*}
$$

for $M_{1}^{ \pm}=700 \mathrm{GeV}$.
At the LHC, the typical cross sections for $V_{i}$ are hundreds of femtobarns, so, after cuts, the LHC experiments will record tens to hundreds of events in the first years of data taking. Since the $V_{i}$ resonances serve the same purpose as the Higgs boson, additional information will be necessary to determine whether these resonances originate from spontaneous symmetry breaking or from strong coupling between the known gauge bosons. The electroweak measurements from NuSOnG will play a role in understanding the origin of such events, en route to a more complete explanation provided by the ILC.

### 2.2 The NuTeV Anomaly

The NuTeV anomaly is a $3 \sigma$ deviation of $\sin ^{2} \theta_{W}$ from the Standard Model prediction 4. NuTeV employed the PW-inspired method discussed in Sec. 2.1.1.1, which resulted in a $0.75 \%$ measurement of the weak mixing angle (see Tab. 11). Two systematic adjustments to the NuTeV result have been identified since the result was published. The first is the new measurement of the $K_{e 3}$ branching ratio from KTeV , which does not significantly reduce the error, but introduces a correction moving the result away from the Standard Model. The second is the final measurement of the difference between the strange and antistrange seas (called "the strange sea asymmetry", see Sec. 2.4.4., which will pull the NuTeV result toward the Standard Model. A new analysis of the NuTeV data which will include these two corrections is expected be available in late summer, 2007 [32]. It should be noted that while an error from the strange sea appeared in the NuTeV analysis, no error on a strange sea asymmetry appeared in the original NuTeV analysis; this will be included in the upcoming re-analysis.

NuTeV is one of a set of $Q^{2} \ll m_{Z}^{2}$ experiments measuring $\sin ^{2} \theta_{W}$. It was performed at $Q^{2}=1$ to $140 \mathrm{GeV}^{2},\left\langle Q_{\nu}^{2}\right\rangle=26 \mathrm{GeV}^{2},\left\langle Q_{\bar{\nu}}^{2}\right\rangle=15 \mathrm{GeV}^{2}$, which is also the expected range for NuSOnG. Two other precision low $Q^{2}$ measurements are from atomic parity violation [34] (APV), which samples $Q^{2} \sim 0$; and SLAC E158, a Møller scattering experiment at average $Q^{2}=0.026 \mathrm{GeV}^{2}$ [35]. Using the measurements at the $Z$-pole with $Q^{2}=M_{z}^{2}$ to fix the value of $\sin ^{2} \theta_{W}$, and evolving to low $Q^{2}$, Fig. 4 from ref. [31], shows that APV and SLAC E158 are in agreement with the Standard Model. However, the radiative corrections to neutrino interactions allow sensitivity to highmass particles which are complementary to the APV and Møller-scattering corrections. Thus, these results may not be in conflict with NuTeV . The NuSOnG measurement will provide valuable additional information on this question.

Since the NuTeV result was published, more than 300 papers have been written which cite this result. Various Beyond-the-Standard-Model explanations have been put forward; those which best explain the result require a follow-up experiment which probes the neutral weak couplings specifically with neutrinos, such as NuSOnG. Several "within-Standard-Model" explanations have also been put forward, based on the inherent issues involving scattering off quarks. NuSOnG can address these criticisms in two ways. First, we will provide better constraints of the quark-related distributions at issue. Second, we perform the measurement of the weak mixing angle in both a


Figure 4: Measurements of $\sin ^{2} \theta_{W}$ as a function of $Q$; from ref. [31]. The curve shows the Standard Model expectation.
purely leptonic mode (scattering from electrons) and via the PW method. Agreement between the two results would address the questions which have been raised.

### 2.2.1 Explanations Within the Standard Model

Four explanations for the NuTeV anomaly that are "within the Standard Model" have been proposed. These are: electromagnetic radiative corrections; higher order QCD corrections; isospin (or charge symmetry) violation; and the strange sea asymmetry. The radiative corrections will be disregarded here, since the results of this paper 36] are not reproducible.

The effect of the possible explanations is illustrated in Fig. 5. On this plot, the solid horizontal line indicates the deviation of NuTeV from the Standard Model. The thick vertical lines, which emanate from the NuTeV deviation, show the range of pulls estimated for each explanation, as discussed below. The dashed horizontal line shows the estimated shift due the new $K_{e 3}$ branching ratio. We do not yet have an estimated shift due to the new NuTeV strange sea measurement, but it is expected that this will move the dashed line toward the Standard Model [32].

Three "Standard Model" explanations may be considered next [37, 38]. First, the NuTeV analysis was not performed at a full NLO level; NuSOnG will need to undertake a full NLO analysis. But the effect of going to NLO on NuTeV can be estimated [39], and the expected pull is away from the Standard Model, as shown on Fig. 5. Second, the NuTeV analysis assumed isospin symmetry, that is, $u(x)^{p}=d(x)^{n}$ and $d(x)^{p}=u(x)^{n}$. Isospin violation can come about from a variety of sources and is interesting in its own right. NuSOnG's contribution to this study is discussed in Section 2.4.3. Various models for isospin violation have been studied and their pulls range from less than $1 \sigma$ away from the Standard Model to $\sim 1 \sigma$ toward the Standard Model [40]. We have chosen three examples [40] for illustration on Fig. 5 the full bag model, the meson cloud model, and the isospin QED model. These are mutually exclusive models, so only one of these can affect the NuTeV anomaly. Third, variations in the predicted strange sea asymmetry can either pull the result toward or away from the Standard Model expectation [41, 42, 43]. This issue is considered in detail in Sec. 2.4.4.

### 2.2.2 Beyond Standard Model Interpretations

Chapter 14 of the APS Neutrino Study White Paper on Neutrino Theory [44] is dedicated to "the physics of NuTeV" and provides an excellent summary. The discussion presented here is drawn from this source.

The NuTeV measurements of $R^{\nu}$ and $R^{\bar{\nu}}$, the NC-to-CC cross sections, are low. If one is assumes that the Higgs is light, then this must be interpreted as Beyond-Standard-Model physics that suppresses the NC rate with respect to the CC rate. Two types of models produce this effect and remain consistent with the other electroweak measurements: 1) models which affect only the $Z$ couplings, e.g., the introduction of a heavy $Z^{\prime}$ boson which interferes with the Standard Model $Z$; or 2) models which affect only the neutrino couplings, e.g., the introduction of moderate mass neutral heavy leptons which mix with the neutrino.

As discussed in Sec. 2.1.2.4, introduction of $Z^{\prime}$ bosons tend to increase the NC rate rather than suppress it. Thus there is only a small subset of models which produce the destructive interference needed to explain the NuTeV result. Models which introduce


Figure 5: Effect of various "Standard Model" explanations on the NuTeV anomaly. The $y$-axis is the deviation from the Standard Model. The solid line is the NuTeV deviation. The dashed line is an estimate of the effect of correcting for the new $K_{e 3}$ branching ratio. Thick black lines extending from the NuTeV deviation show the range of possible pulls from the various suggested sources, as described in the text.
a $Z^{\prime}$ which selectively suppresses neutrino scattering, without significantly affecting the other electroweak measurements, include cases where the $Z^{\prime}$ couples to $B-3 L_{\mu}$ [45] or to $L_{\mu}-L_{\tau}$ [46]. In the former case, fitting the NuTeV anomaly requires that $M_{Z^{\prime}} / g_{Z^{\prime}} \sim 3 \mathrm{TeV}$. From the bounds from direct searches, this sets a limit on $M_{Z^{\prime}}>600$ GeV if the coupling is on the order of unity, but as low as 2 to 10 GeV if the coupling is $\sim 0.1 \%$. The latter case is an example which improves the agreement between NuTeV and other results, but does not entirely address the problem. Its effectiveness in solving the NuTeV anomaly is limited by the data constraining lepton universality. This model addresses more than just the NuTeV anomaly. It is inspired by attempts to address bimaximal mixing in the neutrino sector. It has the nice features of also addressing the muon $(g-2)$ measurement and producing a distinctive dimuon signature at LHC.

The case of models involving moderate-mass neutral heavy leptons, a.k.a. neutrissimos, have been discussed in the Sec. 2.1.2.3 and examples of viable models appear in ref. [11. Eq. 30 described how the muon neutrino couplings might be modified by mixing. This idea can be extended to all three flavors, leading to a suppression factor for the $Z$ coupling which is expressed as $\left(1-\epsilon_{\ell}\right)$ and for the $W$ by $\left(1-\epsilon_{\ell} / 2\right)$, where $\ell=e, \mu$, or $\tau$. This addresses the NuTeV anomaly and at the same time suppresses the invisible width of the $Z$, describing the LEP I data.

If the NuTeV anomaly is due to Beyond Standard Model physics, then the effect will be visible in the neutrino-electron elastic scattering measurement also. Thus, if the NuTeV anomaly is borne out, NuSOnG would observe an $S T$ plot similar to Fig. 6.

### 2.3 Direct Searches for New Physics

### 2.3.1 Light Neutrino Properties

Evidence for three light neutrino masses has now been established through neutrino oscillations in solar, atmospheric, and reactor experiments (see references [47] through [61). Furthermore, although the MiniBooNE experiment recently refuted the LSND two-neutrino oscillation scenario at $\Delta m^{2} \sim 1 \mathrm{eV}^{2}$ [62], the question of the existence of multiple light sterile neutrinos still remains open [63]. These observations already require beyond-the-Standard-Model physics, and consequently raise phenomenological questions, such as: what are the mass and mixing parameters still allowed in sterile neutrino models? What do sterile neutrinos imply about neutrino mixing? Is the neutrino mixing matrix unitary, or is there effective freedom of mixing parameters? As we illustrate in the following sections, these are some of the questions that NuSOnG can potentially address.

### 2.3.1.1 Matrix Freedom

Perhaps the most interesting study of light neutrino properties which can be performed at NuSOnG is the search for evidence of "matrix freedom" or "nonunitarity." For example, in the case of existence of sterile neutrinos, the neutrino mixing matrix is extended to an $N \times N$ matrix, where $N>3$. Under that assumption, it has been suggested that the $3 \times 3$ part of the matrix describing the three active (SM) neutrinos is not necessarily unitary; or, equivalently, the three flavor eigenstates are non-orthogonal (the $3 \times 3$ neutrino mixing matrix is free) [64].


Figure 6: Three projected electroweak measurements from NuSOnG in S-T plane for a model model with a heavy Higgs inspired by the NuTeV measurement [11]. In this model, $(S, T)=(0.12,-0.36)$. The labeling is as in Fig. 3.

This introduces striking changes to the probability formula for neutrino flavor transitions. Assuming unitarity, the survival probability formula for a neutrino produced as flavor $\alpha$ is

$$
\begin{equation*}
P_{\alpha \alpha}^{\text {unitary }}=1-4\left|U_{\alpha 3}\right|^{2}\left[1-\left|U_{\alpha 3}\right|^{2}\right] \sin ^{2} \Delta_{31}, \tag{33}
\end{equation*}
$$

where one has made use of $\Delta_{31}=\Delta m_{31}^{2} \frac{L}{4 E}$, and $\Delta m_{21}^{2} \frac{L}{4 E} \ll 1$. In the case of matrix freedom, the mixing matrix is no longer unitary. The level at which unitarity is violated can be defined as $X_{\alpha}$, where

$$
\begin{equation*}
\sum_{j}\left|U_{\alpha j}\right|^{2}=1-X_{\alpha}, \tag{34}
\end{equation*}
$$

with $X_{\alpha}$ being small. Under that assumption, the survival probability formula is then found to be

$$
\begin{equation*}
P_{\alpha \alpha}^{\text {general }}=P_{\alpha \alpha}^{\text {unitary }}-2 X_{\alpha}\left[1-2\left|U_{\alpha 3}\right|^{2} \sin ^{2} \Delta_{31}\right]+X_{\alpha}^{2} . \tag{35}
\end{equation*}
$$

As implied by Eq. 35 one of the main consequences of such scenario is instantaneous ( $L=0$ ) flavor transitions in a neutrino beam. This occurs regardless of the size of the mass splitting between the mostly sterile and mostly active states, and thus allows for a full-mass-range search for evidence of sterile neutrinos. A recent study [65] suggests that current experimental data limit such an effect to up to the order of a few percent.

As a result, several interesting and potentially observable phenomena can occur. Extending the argument of ref. [65], for instance, the non-orthogonality of $\nu_{\mu}$ and $\nu_{e}$ that matrix freedom introduces, results in an instantaeous transition at $L=0$ from $\nu_{\mu}$ to $\nu_{e}$ [64. Thus one could observe an excess of $\nu_{e}$ events in a pure $\nu_{\mu}$ beam.

The trick to searching for this instantaneous transition is to focus on an energy range where the $\nu_{e}$ background is low and well constrained. In the case of NuSOnG, this is on the high energy tail of the flux, above $\mathrm{E} \gtrsim 250 \mathrm{GeV}$. For the limits on $\nu_{\mu}$ transformation to $\nu_{e}$ [65], which are at the $\sim 1 \times 10^{-4}$ level, NuSOnG would see an excess of $\sim 200 \nu_{e}$ events in this high energy region. Fig. 7 shows the ratio of $\nu_{e}$ flux with $\nu_{\mu}$ transitions to $\nu_{e}$ flux without transitions. The abrupt cutoff is due to Monte Carlo statistics; higher energies can be explored. Assuming that such transitions indeed happen at the $10^{-4}$ level, one would expect up to a $10 \%$ increase in flux for $\mathrm{E} \sim 350$ GeV . In that high energy region, the $\nu_{e}$ flux is mainly from $K^{+}$decay, which is well constrained by the $\nu_{\mu}$ events. Such an excess should therefore be measurable.

Other interesting effects of matrix freedom [64] include the oscillatory behavior in the total (flavor-summed) CC event rate as a function of $L / E$, and (fake) CP-violating effects in the $\nu$ and $\bar{\nu}$ neutral-current event rates (the two rates oscillate differently with $L / E)$. Potential observation of those effects at NuSOnG has not been explicitly considered at this stage, although it would be interesting to address this and we are planning to do so in the near future. Regardless of that, evidence of $\nu_{e}$ contamination in a $\nu_{\mu}$ beam above expected background levels, something for which NuSOnG can search, would strongly support the matrix freedom hypothesis.

### 2.3.1.2 Sterile Neutrino Oscillations

Direct observation of sterile neutrino oscillations may also be possible in NuSOnG, depending on the mass and mixing parameters. Oscillations of active to light sterile neutrinos have been introduced to explain the LSND anomaly, as dark matter candidates, and in describing the supernova collapse models. These ideas span a wide


Figure 7: Ratio of enhanced $\nu_{e}$ flux due to $\nu_{\mu}$ transitions to $\nu_{e}$ flux assuming no transitions. Obtained assuming $100 \mathrm{M} \nu_{\mu}$ deep inelastic scattering events.
range of $\Delta m^{2}$ values. The LSND anomaly requires a sterile neutrino in the range of $\sim 1 \mathrm{eV}^{2}$ with moderate mixing ( $\lesssim 1 \%$ ), while dark matter candidates and supernova collapse models require ( $\gtrsim 1 \mathrm{keV})^{2}$. These models also require tiny mixing $\left(10^{-13}<\sin ^{2} 2 \theta<10^{-7}\right)$ 66]. NuSOnG probes an intermediate range of $\Delta m^{2}$, between the LSND and astrophysical allowed regions. However, since sterile neutrinos may come in families, it is worth exploring this previously uncharted territory.

The NuSOnG experimental design consists of a $30-600 \mathrm{GeV}$ muon neutrino beam, peaked at $\sim 100 \mathrm{GeV}$, incident on a $\sim 200$-meter long detector located at $\mathrm{L} \sim 1.5 \mathrm{~km}$ from the neutrino source. This detector design allows for $\nu_{\mu}$ disappearance studies across the detector length by examining the $\nu_{\mu}$ scattering rate variation across the detector. Such searches would be limited by the detector energy resolution. Preliminary studies have shown that, assuming a $10 \%$ energy resolution, $\Delta m^{2} \sim 600 \mathrm{eV}^{2}$ regions with mixing of $\lesssim 0.1$ can be probed easily. NuSOnG may also be able to explore smaller mixings and higher $\Delta m^{2} \mathrm{~s}$, depending on the final experimental design.

NuSOnG can also probe for $\nu_{\mu}$ and $\nu_{e}$ disappearance in the range of $L / E=$ $(1.5 \mathrm{~km} / 100 \mathrm{GeV})=0.015$, thus in the range of $\Delta m^{2} \sim 50 \mathrm{eV}^{2}$. This is a range which has been covered by past experiments including CCFR [67], CHDS [68], and NOMAD [69]. However, the improved quality of the first principles prediction due to the new SPY secondary production data [70], discussed in sec. 3.3, should allow improvement of these limits.

### 2.3.2 New Interactions

### 2.3.2.1 Lepton Number Violation Searches

The NuSOnG experiment possesses two valuable characteristics for the search for lepton number violation. First, it relies upon a high purity, high intensity beam as
its source of neutrinos; secondly, it employs an instrumented detector optimized to measure inverse muon decay with high accuracy. An experiment with these two features naturally lends itself to searches for the process:

$$
\begin{equation*}
\bar{\nu}_{\mu}+e^{-} \rightarrow \mu^{-}+\bar{\nu}_{e} . \tag{36}
\end{equation*}
$$

This interaction is forbidden by the Standard Model since it violates lepton family number conversation ( $\Delta L_{e}=-\Delta L_{\mu}=2$ ). As such, observation of this reaction would immediately constitute direct observation of physics beyond the Standard Model.

A number of theories beyond the Standard Model predict that lepton number is not a true conserved quantum number; this means that processes that violate lepton number are allowed to occur. Theories which incorporate multiplicative lepton number conservation [71, 72], left-right symmetry [73], or the existence of bileptons [74] fall under this category.

The differential cross-section for lepton-violating processes can be parametrized in the following form:

$$
\begin{equation*}
\frac{d \sigma}{d y}=\lambda \frac{G_{F}^{2} s}{\pi}\left(A_{V} \cdot y(y-r)+A_{S} \cdot(1-r)\right) \tag{37}
\end{equation*}
$$

where $y$ is the fractional energy carried by the outgoing lepton, $G_{F}$ the weak coupling constant, $s$ the square of the center of mass energy of the system, and $r$ the threshold factor, defined as $m_{\mu}^{2} / s$. The parameters $\lambda, A_{V}$, and $A_{S}$ describe the strength of the reaction and whether the process is vector or scalar in nature. It is typical to compare this process to that of inverse muon decay:

$$
\begin{equation*}
\frac{\sigma\left(\bar{\nu}_{\mu} e^{-} \rightarrow \mu^{-} \bar{\nu}_{e}\right)}{\sigma\left(\nu_{\mu} e^{-} \rightarrow \mu^{-} \nu_{e}\right)}=\lambda \cdot\left(A_{V} \cdot\left(\frac{1+r / 2}{3}\right)+A_{S}\right) . \tag{38}
\end{equation*}
$$

The signature for such a reaction is the tagging of an $\mu^{-}$during antineutrino running with the same signature as expected from inverse muon decays. The main backgrounds to this reaction include (a) $\nu_{\mu}$ contamination, (b) $\nu_{e}$ contamination, and (c) charge misidentification of candidate events. Our current estimates place a very small beam contamination during antineutrino running: about $0.4 \%$ contamination of $\nu_{\mu} \mathrm{s}$ and a $2.3 \%$ contamination of $\nu_{e}$ and $\bar{\nu}_{e}$ neutrinos (See Sec. 3.1). Charge misidentification is expected to be very small, on the order of $10^{-5}$. If we assume a conservative knowledge of the backgrounds at the $5 \%$ level, this would imply a limit on the lepton number violation cross-section ratio of better than $0.2 \%$ (at $90 \%$ C.L.) for V-A couplings and less than $0.06 \%$ for scalar couplings. Previous searches, based on $1.6 \times 10^{18}$ protons on target and smaller target masses, have placed limits on this cross-section ratio to less than $1.7 \%$ at $90 \%$ C.L. for V-A couplings and less than $0.6 \%$ for scalar couplings [75]. The NuSOnG experiment can therefore reach an improvement of over an order of magnitude compared to previous searches. This limit can be improved if further selection criteria are used in removing unwanted beam impurities or the quasi-elastic background contamination.

### 2.3.2.2 Inverse Muon Decay

The study of inverse muon decay, $\nu_{\mu}+e^{-} \rightarrow \mu^{-}+\nu_{e}$ provides access to the helicity structure of the weak interaction distinct from muon decay experiments. The weak
interaction polarizes the incident $\nu_{\mu}$, making inverse muon decay an excellent place to study departures from $V-A$ couplings. For inverse muon decay, $\sigma \propto\left(g_{L}^{V, e} g_{L}^{V, \mu}\right)^{2}(1-\epsilon)$ [76] where $\epsilon=h-(-1)$ and $h$ is the helicity of the incident muon. Ref. [77] has measured $\epsilon<4.1 \times 10^{-3}$ and the current limit on $g_{L L}^{V}=\left(g_{L}^{V, e} g_{L}^{V, \mu}\right)>0.96$ [78]. For a measurement of the total cross section scaled to the predicted cross section, the uncertainty on the coupling is $g_{L L}^{V}=(1 / 2) \sigma_{\sigma} / \sigma_{S M}$.

For NuSOnG, we expect $>200 \mathrm{k}$ inverse muon decay events, which would give a statistical uncertainty of 0.002 on $g_{L L}^{V}$. However, we will need to determine the neutrino flux. Taking the $\nu_{\mu}+e^{-} \rightarrow \nu_{\mu}+e^{-}$cross section as known gives the neutrino flux to $0.7 \%$. Since we plan to use the inverse muon decay events for determining the flux for the electroweak measurements, NuSOnG will need to measure the efficiency and fiducial volume for both processes to better than $0.7 \%$. Combined with other systematics, we should be able to achieve an total uncertainty of about $1-2 \%$ on $g_{L L}^{V}$, an improvement by a factor of four.

The key background will come from CCQE events that have small hadronic energy. We expect our high granularity will allow us to keep the systematic error from this source well below $1 \%$, but this needs study.

Obviously, the manner of analysis described above is somewhat questionable. Ultimately, one would want to carry out a combined analysis of both neutrino elastic scattering on electrons and quarks and of inverse muon decay in the context of a specific model which relates the charged and neutral current coupling constants. For such an analysis, $1-2 \%$ uncertainty should still be achievable.

### 2.3.3 New Particles

### 2.3.3.1 Long-lived, Light Neutral Heavy Leptons

Another interesting NuTeV result arose from the search for long-lived, light ( $<15$ GeV ) neutral heavy leptons. This was performed in a helium-filled decay region located upstream of the calorimeter. In the mass region of $2.2-15 \mathrm{GeV}, \mathrm{NuTeV}$ has a small expected background ( $0.07 \pm 0.01$ events), but observed three events. All events had two muons originating from a vertex within the helium decay region and missing energy. [79.

Since publication in 2001, no widely accepted explanation has been found. In 2006, D0 published a search for a similar decay signature in proton-antiproton interactions 80. No events were found and some production models were excluded. The most viable remaining model is by Dedes et al., which hypothesizes that the events are from decay of long-lived neutralinos. These are produced in the NuTeV beam dump through $B$ hadron decays [81]. No other experiment has been able to match NuTeV's running conditions to further explore this intriguing result.

NuSOnG can address the question by including a low-mass (helium-filled) decay region between the calorimeter segments. Assuming parameters similar to those of NuTeV (except for a 20 -fold increase in the number of protons on target), NuSOnG would expect to see 60 events with an expected background of 1-2 events. The sensitivity would scale directly with the decay volume, so the increased length compared to $\mathrm{NuTeV}(26 m \rightarrow \approx 40 \mathrm{~m})$ would increase this to 90 signal events over a $2-3$ event background. Observing no signal would finally settle this outstanding question.

These decay regions allow exploration for a signal from a beyond-the-StandardModel particle in other decay modes as well; other interesting modes include $\mu \pi, \mu e$, $e \pi$ and $e e$. NuSOnG's sensitivity to other new particles is similarly improved over NuTeV by the increase in beam intensity and decay volume, allowing us to study new regions of phase space.

### 2.3.3.2 Muonic Photons

In the mid-1990's there was interest in searching for "leptonic photons" - massless vector particles that couple according to flavor. Electronic, muonic, and tauonic photons, $\gamma_{e}, \gamma_{\mu}$, and $\gamma_{\tau}$ were introduced [82]. Production occurs in secondary meson decays such as $\pi \rightarrow \nu_{\mu} \mu \gamma_{\mu}$, and detection can proceed through $\gamma_{\mu}+Z \rightarrow \mu^{+}+\mu^{-}+Z$, where $Z$ is the charged nucleus. These events have small missing $p_{T}$ compared to the "trident" background, $\nu+Z \rightarrow \nu+\mu^{+} \mu^{-}+Z$. The search by CHARM II sets the best limit at $1.6 \times 10^{-6}$ [83].

Since this time, neutrino oscillations have been confirmed (see references 47] through [61]). This complicates the theory of "muonic photons," since, in this case, lepton flavor-charge is not conserved. As pointed out in reference [82], a theory with a nonconserved charge cannot have massless vector particles and a Coulomb-like potential. It appears very difficult to evade this problem.

Nevertheless, NuSOnG should search for these events. With higher rate and better segmentation than CHARM II, NuSOnG should have sensitivity in the range of $\sim 10^{-7}$. A significant excess would be quite startling.

### 2.4 Measurement of Parton Distribution Functions

The Deeply Inelastic Scattering (DIS) process provides crucial information about the structure of the proton which is used to determine the Parton Distribution Functions (PDFs). For example, in the recent CTEQ6HQ analysis, DIS data accounted for more than two-thirds of the data points used in the analysis 11 As such, the DIS measurements form the foundation for the many calculations which make use of the PDFs.

In the basic DIS process, leptons scatter from hadrons via the exchange of an intermediate vector boson: $\left\{\gamma, W^{ \pm}, Z\right\}$. Different boson probes couple to the hadrons with different factors, and it is important to combine data from these different probes to separate the different flavor components in the hadron. Unfortunately, three of the four DIS probes $\left\{W^{ \pm}, Z\right\}$ have a (relatively) large mass and couple only weakly; this introduces a number of complications:

- The statistics for these weak processes are limited as compared with the photonexchange processes.
- To compensate for the weak cross section, typically heavy nuclear targets (e.g., Fe and Pb ) are used; this introduces nuclear corrections when the results are scaled from the heavy target back to proton or isoscalar targets.

The NuSOnG experiment will generate high statistics ( $>100 \mathrm{M}$ DIS events) measurements on an intermediate atomic-weight nuclear target $\left(\mathrm{SiO}_{2}\right)$. This will provide

[^290]precise information on the linear combinations of PDFs which couple to the weak charged currents ( $W^{ \pm}$), which can significantly improve the parton distribution fits. In this section, we first introduce the basics of DIS and the connection to parton distribution functions. Then we concentrate on three aspects of parton distribution studies where NuSOnG can make a unique contribution to the physics:

- Improved understanding of nuclear effects in neutrino scattering.
- Study of Charge Symmetry Violation
- Measurement of the Strange Sea
- Measurement of $\sigma^{\nu}$ and $\sigma^{\bar{\nu}}$

The latter two items are directly relevant to the electroweak studies proposed for NuSOnG (see Sec. 2.2.1).

### 2.4.1 Deep Inelastic Scattering and Parton Distribution Functions

The differential cross section for neutrino DIS depends on three structure functions: $F_{2}, x F_{3}$ and $R_{L}$. It is given by:

$$
\begin{align*}
\frac{d^{2} \sigma^{\nu(\bar{\nu}) N}}{d x d y}= & \frac{G_{F}^{2} M E_{\nu}}{\pi\left(1+Q^{2} / M_{W}^{2}\right)^{2}} \\
& {\left[F_{2}^{\nu(\bar{\nu}) N}\left(x, Q^{2}\right)\left(\frac{y^{2}+(2 M x y / Q)^{2}}{2+2 R_{L}^{\nu(\bar{\nu}) N}\left(x, Q^{2}\right)}+1-y-\frac{M x y}{2 E_{\nu}}\right)\right.} \\
& \left. \pm x F_{3}^{\nu(\bar{\nu}) N} y\left(1-\frac{y}{2}\right)\right] \tag{39}
\end{align*}
$$

where the $\pm$ is $+(-)$ for $\nu(\bar{\nu})$ scattering. In this equation, $x$ is the Bjorken scaling variable, $y$ the inelasticity, and $Q^{2}$ the squared four-momentum transfer.

The function $x F_{3}\left(x, Q^{2}\right)$ is unique to the DIS cross section for the weak interaction. It originates from the parity-violating term in the product of the leptonic and hadronic tensors. For an isoscalar target, in the quark-parton model,

$$
\begin{align*}
x F_{3}^{\nu N}(x)= & x(u(x)+d(x)+2 s(x)  \tag{40}\\
& -\bar{u}(x)-\bar{d}(x)-2 \bar{c}(x)), \\
x F_{3}^{\bar{\nu} N}(x)= & x F_{3}^{\nu N}(x)-4 x(s(x)-c(x)) . \tag{41}
\end{align*}
$$

Defining $x F_{3}=\frac{1}{2}\left(x F_{3}^{\nu N}+x F_{3}^{\bar{\nu} N}\right)$, at leading order in QCD,

$$
\begin{equation*}
x F_{3, L O}=\sum_{i=u, d . .} x q\left(x, Q^{2}\right)-x \bar{q}\left(x, Q^{2}\right) . \tag{42}
\end{equation*}
$$

To the level that the sea quark distributions have the same $x$ dependence, and thus cancel, $x F_{3}$ can be thought of as probing the valence quark distributions. The difference between the neutrino and antineutrino parity violating structure functions, $\Delta\left(x F_{3}\right)=$ $x F_{3}^{\nu N}-x F_{3}^{\bar{\nu} N}$, probes the strange and charm seas.

Analogous functions for $F_{2}\left(x, Q^{2}\right)$ and $R_{L}\left(x, Q^{2}\right)$ appear in both the cross section for charged lepton ( $e$ or $\mu$ ) DIS and the cross section for $\nu$ DIS. At leading order,

$$
\begin{equation*}
F_{2, L O}=\sum_{i=u, d . .} e^{2}\left(x q\left(x, Q^{2}\right)+x \bar{q}\left(x, Q^{2}\right)\right), \tag{43}
\end{equation*}
$$

where $e$ is the charge associated with the interaction. In the weak interaction, this charge is unity. For charged-lepton scattering mediated by a virtual photon, the fractional electromagnetic charge of each quark flavor enters. Thus $F_{2}^{\nu N}$ and $F_{2}^{e(\mu) N}$ are analogous but not identical and comparison yields useful information about specific parton distributions 87. $R_{L}\left(x, Q^{2}\right)$ is the longitudinal to transverse virtual boson absorption cross-section ratio. The best measurements for this come from charged lepton scattering rather than neutrino scattering. In the past, neutrino experiments have used the charged lepton fits to $R_{L}$ as an input to the measurements of $x F_{3}$ and $F_{2}[85]$. This, however, is just a matter of the statistics needed for a global fit to all of the unknown structure functions in $x$ and $Q^{2}$ bins [86]. With the high statistics of NuSOnG, precise measurement of $R_{L}$ will be possible from neutrino scattering for the first time.

In addition to fitting to the inclusive DIS sample, neutrino scattering can also probe parton distributions through exclusive samples. A unique and important case is the measurement of the strange sea through opposite sign dimuon production. When the neutrino interacts with an $s$ or $d$ quark, it produces a charm quark that fragments into a charmed hadron. The charmed hadron's semileptonic decay (with branching ratio $B_{c} \sim 10 \%$ ) produces a second muon of opposite sign from the first:

$$
\begin{align*}
\nu_{\mu}+\mathrm{N} \longrightarrow \mu^{-}+ & c+\mathrm{X}  \tag{44}\\
& \hookrightarrow s+\mu^{+}+\nu_{\mu} . \tag{45}
\end{align*}
$$

Similarly, with antineutrinos, the interaction is with an $\bar{s}$ or $\bar{d}$,

$$
\begin{align*}
\bar{\nu}_{\mu}+\mathrm{N} \longrightarrow \mu^{+}+ & \bar{c}+\mathrm{X}  \tag{46}\\
& \hookrightarrow \bar{s}+\mu^{-}+\bar{\nu}_{\mu} . \tag{47}
\end{align*}
$$

The opposite sign of the two muons can be determined for those events where both muons reach the toroid spectrometer. Study of these events as a function of the kinematic variables allows extraction of the strange sea, the charm quark mass, the charmed particle branching ratio $\left(B_{c}\right)$, and the Cabibbo-Kobayashi-Maskaka matrix element, $\left|V_{c d}\right|$.

For a more in-depth review of precision measurement of parton distributions in neutrino scattering, see ref. [88].

### 2.4.2 Nuclear Effects

Historically, neutrino experiments have played a major role in expanding our understanding of parton distribution functions through high statistics experiments such as CCFR [85], NuTeV [89, and CHORUS [90]. However, the high statistics extract a price since the large event samples require the use of nuclear targets - iron in the case of both CCFR and NuTeV and lead in the case of the Chorus experiment. The problem is that if one wants to extract information on nucleon PDFs, then the effects of the nuclear targets must first be removed. NuSOnG can provide key measurements which will improve these corrections.

In the case of charged lepton deep inelastic scattering, there are data available from nuclear targets covering the range from deuterium through iron and beyond. Thus, it has been possible to perform detailed studies of the $A$-dependence as a function of $x$ and $Q^{2}$ from both the cross section and the structure function $F_{2}$. Such is not the case
in $\nu$ and $\bar{\nu}$ interactions where the corrections can be different for both cross sections or, equivalently, for $F_{2}$ and $x F_{3}$. In this case one must rely on theoretical models of the nuclear corrections. This is an unsatisfactory situation since one is essentially measuring quantities sensitive to the convolution of the the desired PDFs and unknown - or model dependent - nuclear corrections.

It is important to address the question of nuclear effects in neutrino scattering so that the neutrino data can be used in fits without bringing in substantial uncertainties. For example, in a recent analysis [91] the impact of new neutrino data on global fits for PDFs was assessed. The conclusion reached in this analysis was that the uncertainties associated with nuclear corrections precluded using the neutrino data to constrain the nucleon PDFs. If this uncertainty is addressed, the neutrino data will be a powerful addition to these fits.

Furthermore, nuclear effects are interesting in their own right. Comparison of the charged and neutral lepton scattering data can provide clues to the sources of the major features which appear in nuclear effects: shadowing, antishadowing, and the EMC effect. There is phenomenological evidence which suggests that the nuclear corrections for the $\nu$ and $\bar{\nu}$ cross sections might be rather similar and, in both cases, somewhat smaller than the corresponding corrections in charged lepton deep inelastic scattering. These latter two observations differ from the pattern suggested by the theoretical model 92 for nuclear corrections used in the analysis.

Fig. 8 shows some results from Ref. [91] in the form of "data/theory" averaged over $Q^{2}$ and presented versus $x$. The results are from a global fit but are plotted without the model-dependent nuclear corrections which were used in the fits. What is striking is the similarity of the $\nu$ and $\bar{\nu}$ results, and the overall pattern of deviations, similar to that seen in charged lepton DIS, although the deviations from unity are somewhat smaller. It is interesting to note that there is no clear indication of the turnover at low $x$ which is observed in charged lepton scattering, called shadowing. However, this may be due to kinematic limits of the measurements.

To make progress in understanding nuclear corrections in neutrino interactions, access to high-statistics data on a variety of nuclear targets will be essential. This will allow the $A$-dependence to be studied as a function of both $x$ and $Q^{2}$, as has been done in charged lepton deep inelastic scattering. PDFs from global fits without the neutrino data can then be used to make predictions to be compared with the $A$-dependent $\nu$ and $\bar{\nu}$ cross sections, thereby allowing the nuclear corrections to be mapped out for comparison with theoretical models.

The primary target of NuSOnG will be $\mathrm{SiO}_{2}$. However, we can address this issue by replacing a few slabs of glass with alternative target materials: $\mathrm{C}, \mathrm{Al}, \mathrm{Fe}$, and Pb . This range of nuclear targets would both extend the results of Miner $\nu$ a to the NuSOnG kinematic region, and provide a check (via the Fe target) against the NuTeV measurement.

Given the NuSOnG neutrino flux, we anticipate $58 k \nu$-induced and $30 k \bar{\nu}$-induced CC DIS events per ton of material. A single ton would be sufficient to extract $F_{2}(x)$ and $x F_{3}(x)$ averaged over all $Q^{2}$; a single $5 \mathrm{~m} \times 5 \mathrm{~m} \times 2.54 \mathrm{~cm}$ slab of any of the above materials will weigh more than that. The use of additional slabs would permit further extraction of the structure functions into separate $\left(x, Q^{2}\right)$ bins as was done in the NuTeV analysis, at the potential expense of complicating the shower energy resolution in the sub-detectors containing the alternative targets; this issue will be studied via


Figure 8: Comparison between the reference fit and the unshifted Chorus and NuTeV neutrino data without any nuclear corrections.

| Material | Mass of <br> 2.54 cm slab (tons) | Number of slabs needed <br> for NuTeV-equivalent statistics |
| :---: | :---: | :---: |
| C | 1.6 | 33 |
| Al | 1.9 | 27 |
| Fe | 5.5 | 10 |
| Pb | 7.9 | 7 |

Table 2: Alternative target materials for cross-section analysis
simulation.
Table 2 shows that two 50 -module stacks would be sufficient to accumulate enough statistics on alternative nuclear targets for a full structure-function extraction for each material. However, for basic cross-section ratios in $x$, a single slab of each would suffice.

### 2.4.3 Isospin Violations

When we relate DIS measurements from heavy targets such as ${ }_{26}^{56} \mathrm{Fe}$ or ${ }_{82}^{207} \mathrm{~Pb}$ back to a proton or isoscalar target, we generally make use of isospin symmetry where we assume that the proton and neutron PDFs can be related via a $u \leftrightarrow d$ interchange. While isospin symmetry is elegant and well-motivated, the validity of this exact charge symmetry must ultimately be established by experimental measurement. There have been a number of studies investigating isospin symmetry violation [93, 94, 95, 96; therefore, it is important to be aware of the magnitude of potential violations of isospin symmetry and the consequences on the extracted PDF components. For example, the naive parton model relations are modified if we have a violation of exact $p \leftrightarrow n$ isospinsymmetry, (or charge symmetry); e.g., $u_{n}(x) \not \equiv d_{p}(x)$ and $u_{p}(x) \not \equiv d_{n}(x)$.

Combinations of structure functions can be particularly sensitive to isospin violations, and NuSOnG is well suited to measure some of these observables. For example, residual $u, d$-contributions to $\Delta x F_{3}=x F_{3}^{\nu}-x F_{3}^{\bar{\nu}}$ from charge symmetry violation (CSV) would be amplified due to enhanced valence components $\left\{u_{v}(x), d_{v}(x)\right\}$, and because the $d \rightarrow u$ transitions are not subject to slow-rescaling corrections which strongly suppress the $s \rightarrow c$ contribution to $\Delta x F_{3}$. 95] Here the ability of NuSOnG to separately measure $x F_{3}^{\nu}$ and $x F_{3}^{\bar{\nu}}$ over a broad kinematic range will provide powerful constraints on the sensitive structure function combination $\Delta x F_{3}$.

There are a wide variety of models that study CSV [93, 94, 95, 96]. One method to quantify possible CSV contributions is via a one-parameter "toy" model where we characterize the CSV as a rotation in isospin space: $q_{n}^{\mathrm{CSV}}=N_{q} \sum_{q^{\prime}} R_{q q^{\prime}}(\theta) q_{p}^{\prime}$, where $R$ is a rotation matrix, and $N_{q}$ is the normalization factor. For example, the $u$-distribution in the neutron can be related to the proton distributions via:

$$
\begin{equation*}
u_{n}^{\mathrm{CSV}}\left(x, Q^{2}\right)=N_{u}^{2}\left[\cos ^{2}(\theta) u_{p}\left(x, Q^{2}\right)+\sin ^{2}(\theta) d_{p}\left(x, Q^{2}\right)\right] . \tag{48}
\end{equation*}
$$

For $\theta=\pi / 2$, we recover the symmetric limit $u_{p}\left(x, Q^{2}\right)=d_{n}\left(x, Q^{2}\right)$. While this parameterization does not offer any explanation for the source of the CSV, it does provide a simple one-parameter $(\theta)$ characterization which is flexible enough to quantify the range of CSV effects. (For more details, cf. Ref. 95].)

At present, there are constraints on isospin violation from a number of experiments which cover different ranges of $x$ and $Q^{2}$. For example, we note that while the above
"toy" model leaves the neutron singlet combination $(q+\bar{q})$ invariant at the $\lesssim 2 \%$ level in the region $x \epsilon[0.01 ; 0.1]$, it would lower the NC observable $\left[\frac{4}{9}(u+\bar{u})+\frac{1}{9}(d+\bar{d})\right]_{n}$ in this region by about $10 \%$. An effect of this size would definitely be visible in the NMC $F_{2}^{n} / F_{2}^{p}$ data which has an uncertainty of order a few percent. 87] The measurement of the lepton charge asymmetry in W decays from the Tevatron [97, 98] places tight constraints on the up and down quark distributions in the range $0.007<x<0.24$. While only strictly telling us about parton distributions in the proton, these data rule out isospin violations at the $5 \%$ level, as demonstrated in Ref. [98. In addition, there are also fixed-target Drell-Yan experiments such as NA51 [99] and E866 [100] which precisely measure $\bar{d} / \bar{u}$ in the range $0.04<x<0.27$; these are also sensitive to isospin-violating effects.

NuSOnG will be able to provide high statistics DIS measurements across a wide $x$ range. Because the target material $\left(\mathrm{SiO}_{2}\right)$ is very nearly isoscalar, this will essentially allow a direct extraction of the isoscalar observables. Consequently, if isospin violations are present, they can be measured more precisely than would be the case on a highly non-isoscalar target.

### 2.4.4 Measurement of the Strange Sea

There are several reasons why an improved measurement of the strange sea is of interest. First, it contributes to the low- $Q^{2}$ properties of the nucleon in the nonperturbative regime - a question of practical as well as intellectual interest, since many precision oscillation experiments are being performed in the 1 to 20 GeV (hence, nonperturbative) range. It is critical for charm production which provides an important testing ground for NLO QCD calculations. In addition, understanding the threshold behavior associated with the heavy charm mass is of interest to future neutrino experiments.

Distinguishing the difference between the $s(x)$ and $\bar{s}(x)$ distributions,

$$
\begin{equation*}
x s^{-}(x) \equiv x s(x)-x \bar{s}(x), \tag{49}
\end{equation*}
$$

is even more important, and poses additional challenges. First, it is of intrinsic interest in nucleon structure models [43, 38, 37, 101, 102]. Second, the integrated strange sea asymmetry,

$$
\begin{equation*}
S^{-} \equiv \int_{0}^{1} s^{-}(x) d x, \tag{50}
\end{equation*}
$$

has important implications for the precision measurement of the weak mixing angle in deep inelastic scattering of neutrinos ( $c f$. Sec. 2.2 and references [41, 43, 37, 38, [41, 101, 42]). This was not recognized at the time of the $\mathrm{NuTeV} \sin ^{2} \theta_{W}$ publication; an error due to $S^{-}$will be included in the NuTeV reanalysis, to be presented in late summer 2007 [32].

Historically, information on the $s(x)$ and $\bar{s}(x)$ distributions was derived from inclusive cross sections for neutral and charged current DIS via $\Delta\left(x F_{3}\right)$. These analyses made the implicit assumption that the $s(x)$ and $\bar{s}(x)$ seas had the same distribution in $x$. Because the strange sea is relatively small compared to the dominant $u(x)$ and $d(x)$ processes, the resulting uncertainties on the strange sea components were large. For example, the strangeness content of the nucleon, as measured by the momentum fraction carried by $s$ or $\bar{s}$, is of order $3 \%$ at $Q=1.5 \mathrm{GeV}$. For this reason, the strange PDF was typically parametrized using the ansatz $s(x)=\bar{s}(x)=\kappa(\bar{u}+\bar{d}) / 2$, where $\kappa$ measured the deviation from $S U(3)$ flavor symmetry at some low value of $Q$.


Figure 9: $\quad x s^{-}(x)$ vs $x$ at $Q^{2}=16 \mathrm{GeV}^{2}$. Outer band is combined errors, inner band is without $B_{c}$ uncertainty.

Introducing information from opposite sign dimuon production allows substantial improvement in the strange PDF measurement. Neutrino-induced dimuon production, $(\nu / \bar{\nu}) N \rightarrow \mu^{+} \mu^{-} X$, proceeds primarily through the sub-processes $W^{+} s \rightarrow c$ and $W^{-} \bar{s} \rightarrow \bar{c}$ (respectively), so this provides a mechanism to directly probe the $s(x)$ and $\bar{s}(x)$ distributions without being overwhelmed by the larger $u(x)$ and $d(x)$ distributions. Hence, the recent high-statistics dimuon measurements [103, 104, 105, 106, 107] play an essential role in constraining the strange component of the proton.

The highest precision study of $s^{-}$to date is from the NuTeV experiment [108]. The sign selected beam allowed measurement of the strange and antistrange seas independently, recording 5163 neutrino-induced dimuons, and 1380 antineutrino-induced dimuon events in its iron target. Figure 9 shows the measured asymmetry between the strange and antistrange seas. With more than 100 times the statistics of NuTeV , NuSOnG will have substantially finer binning.

The integrated strange sea asymmetry from NuTeV has a positive central value: $0.00196 \pm 0.00046$ (stat) $\pm 0.00045$ (syst) ${ }_{-0.00107}^{+0.00148}$ (external). The "external" error on the measurement is dominated by the error on the average charm semi-muonic branching ratio, $B_{c}$ which is determined by other experiments. This error currently is about $10 \%$. A rescan of Chorus data, which would increase the statistics, is under consideration [109].

The key to an improved result on the strange sea from NuSOnG is in a more precise measurement of $B_{c}$ at NuSOnG energies. This can be accomplished in two ways. First, the very high statistics of NuSOnG allow for an accurate fit to $B_{c}$ and the $s$ and $\bar{s}$


Figure 10: World measurements of $B_{c}$.
distributions simultaneously. Second, we plan to incorporate an emulsion detector into the design. The emulsion will be scanned by the Nagoya University group. This group has substantial expertise, having provided the emulsion and scanning for Chorus, DoNuT and other emulsion-based experiments. The goal will be to obtain $>10 \mathrm{k}$ events in the emulsion during the NuSOnG run.

Beyond this, we will also consider placing a liquid argon TPC of similar size to microBooNE [110] (70 tons fiducial volume) or even Gargamelle ( 20 tons fiducial volume) in the gap between two of the NuSOnG subdetectors to directly measure $B_{c}$. If one were to, for example, use a volume comparable to the Gargamelle bubble chamber, we could observe on the order of one million charged current events within it for $5 \times 10^{19}$ POT. This would yield approximately 100,000 events with charm in the final state, and about 10,000 dimuon events.

In addition to an improved measurement of $B_{c}$, the more finely-grained liquid argon TPC and/or emulsion detectors could be used to aid the calibration of the four glass detector modules by measuring any differences between hadron and electron showers from pion and electron beams versus those within a neutrino induced event. Coupled with the precision test beam, it may also be possible to improve understanding of the background due to muons produced by pion and kaon decays in the hadron shower. An improved parameterization of this background, currently from a CCFR measurement [111, 112, 113] could help extend the kinematic range of charmed dimuon measurements beyond what was possible for the NuTeV and CCFR experiments.

### 2.4.5 Measurement of the Total Cross Section

Precision measurement of the total neutrino and antineutrino cross sections at high energies will be valuable to a future neutrino factory experiment which seeks to make


Figure 11: World measurements of the total $\nu$ and $\bar{\nu}$ cross sections. See references [89] and [114] through [128].
precision measurement of CP violation. Because NuSOnG can measure the flux to $0.5 \%$ (see Sec. 3.3, precise measurements can be made. Also, higher accuracy on the ratio of $\sigma^{\bar{\nu}} / \sigma^{\nu}$ will also improve the electroweak measurement (see Tab,1).

Fig. 11 shows $\sigma / E_{\nu}$ for the muon neutrino and antineutrino charged-current total cross-section as a function of neutrino energy ([89] and [114]-[128]). The error bars include both statistical and systematic errors. The results are from a wide range of target materials, but the experiments with the smallest errors and largest energy range used iron. The straight lines are the isoscalar-corrected total cross-section values averaged over $30-200 \mathrm{GeV}$ as measured by the experiments in Refs. [115] to [117. The fit [129] gives: $\sigma^{\nu I s o} / E_{\nu}=(0.677 \pm 0.014) \times 10^{-38} \mathrm{~cm}^{2} / \mathrm{GeV} ; \sigma^{\bar{\nu} I s o} / E_{\bar{\nu}}=(0.334 \pm$ $0.008) \times 10^{-38} \mathrm{~cm}^{2} / \mathrm{GeV}$. The average ratio of the antineutrino to neutrino crosssection in the energy range $30-200 \mathrm{GeV}$ is $\sigma^{\bar{\nu}}$ Iso $/ \sigma^{\nu}$ Iso $=0.504 \pm 0.003$ as measured by Refs. [89] and [114]-[117]. Note the change in the energy scale at 30 GeV .

The most precise measurements are systematics limited. The largest contributions to the systematics in recent experiments (CCFR, NuTeV ) come from flux normalization, the model parameterization used in determination of the flux, and the charm mass used to parameterize charm threshold. NuSOnG measures the neutrino flux normalization to high precision via the IMD events. Also, as discussed in Sec. 3.3.2, NuSOnG's high statistics allow cuts which substantially improve the model parameterization error. Lastly, the charm mass, $m_{c}$ is expected to be improved from the high statistics fits to the opposite sign dimuon events described in the previous section. While more study is needed, it likely that NuSOnG can substantially improve on the world measurements of the total cross section and the cross section ratios.


Figure 12: NuSOnG flux in neutrino mode (left) and antineutrino mode (right). Black: muon neutrino flux, red: muon antineutrino flux, blue: electron neutrino and antineutrino flux

## 3 Neutrino Flux and Event Rates

### 3.1 The Neutrino Flux

For the purposes of this expression of interest, we assume the same SSQT design as was used at NuTeV . The resulting neutrino (antineutrino) flux [33] is shown in Fig. 12 , left (right). The $\nu_{\mu}$ flux is shown in black, $\bar{\nu}_{\mu}$ in red, and $\nu_{e}+\bar{\nu}_{e}$ in blue. The shape of the flux is dominated by the dichromatic neutrino spectrum from $\pi$ and $K$ two-body decay.

In neutrino mode, $98.2 \%$ of neutrino interactions are due to $\pi^{+}$and $K^{+}$secondaries, while in antineutrino mode $97.3 \%$ come from $\pi^{-}$and $K^{-}$. The "wrong sign" content is very low, with an $0.03 \%$ antineutrino contamination in neutrino mode and $0.4 \%$ neutrino contamination in antineutrino mode. The electron-flavor content is $1.8 \%$ in neutrino mode and $2.3 \%$ in antineutrino mode. The major source of these neutrinos is
$K_{e 3}^{ \pm}$decay, representing $1.7 \%$ of the total flux in neutrino mode, and $1.6 \%$ in antineutrino mode. Other contributions come from $K_{L e 3}, K_{S e 3}$, charmed meson, muon, $\Lambda_{C}$, $\Lambda$, and $\Sigma$ decays.

Precise knowledge of the electron-flavor content is crucial for many NuSOnG analyses. The largest source of error in the knowledge of the electron-flavor content in NuTeV was from the $K_{e 3}^{ \pm}$branching ratio, which led to an error on $\nu_{e}$ content of $1.4 \%$ [33]. While the other sources of $\nu_{e}$ s have large fractional errors, they constitute a much smaller fraction of the flux. An error of $1.5 \%$ for the electron-flavor contamination, consistent with NuTeV, will be assumed for NuSOnG.

### 3.2 Event Rates

The approximate event rates presented here serve to set the scale for the physics case presented in this document. They are based on running the Nuance event generator [130] with the NuTeV flux, and then scaling to the expectations of NuSOnG assuming a 3 kton fiducial mass. Some simplifying assumptions, which will be corrected as the simulation develops, have been made. For example, $\mathrm{C}_{2}$ is used as a target rather than $\mathrm{SiO}_{2}$. Also, note that Nuance is not yet tuned as a high energy event generator. Thus, these event rates are only representative.

For neutrino running, approximate event rates for $5 \times 10^{19}$ protons are:

| $507 k$ | $\nu_{\mu}$ CC quasi - elastic scatters |
| ---: | :--- |
| $178 k$ | $\nu_{\mu}$ NC - elastic scatters |
| $1016 k$ | $\nu_{\mu} \mathrm{CC} \pi^{+}$ |
| $302 k$ | $\nu_{\mu} \mathrm{CC} \pi^{0}$ |
| $272 k$ | $\nu_{\mu}$ NC $\pi^{0}$ |
| $226 k$ | $\nu_{\mu}$ NC $\pi^{ \pm}$ |
| $1379 k$ | $\nu_{\mu}$ CC and NC Resonance multi - pion |
| $202 M$ | $\nu_{\mu}$ CC Deep Inelastic Scattering |
| $63 M$ | $\nu_{\mu}$ NC Deep Inelastic Scattering |
| $24 k$ | $\nu_{\mu}$ neutrino - electron NC elastic scatters |
| $235 k$ | $\nu_{\mu}$ neutrino - electron CC quasielastic scatters (IMD) |

For antineutrino running, which assumes $1.5 \times 10^{20}$ protons on target, approximate event rates are:

| $548 k$ | $\bar{\nu}_{\mu}$ CC quasi - elastic scatters |
| ---: | :--- |
| $195 k$ | $\bar{\nu}_{\mu}$ NC - elastic scatters |
| $1103 k$ | $\bar{\nu}_{\mu}$ CC $\pi^{+}$ |
| $321 k$ | $\bar{\nu}_{\mu}$ CC $\pi^{0}$ |
| $297 k$ | $\bar{\nu}_{\mu}$ NC $\pi^{0}$ |
| $246 k$ | $\bar{\nu}_{\mu}$ NC $\pi^{ \pm}$ |
| $1516 k$ | $\bar{\nu}_{\mu}$ CC and NC Resonance multi - pion |
| $102 M$ | $\bar{\nu}_{\mu}$ CC Deep Inelastic Scattering |
| $36 M$ | $\bar{\nu}_{\mu}$ NC Deep Inelastic Scattering |

```
21k }\mp@subsup{\overline{\nu}}{\mu}{}\mathrm{ neutrino - electron NC elastic scatters
    0k }\mp@subsup{\overline{\nu}}{\mu}{}\mathrm{ neutrino - electron CC quasielastic scatters (IMD)
```

The above were run for $\nu_{\mu}$ and $\bar{\nu}_{\mu}$ beams. The relative ratios of event-weighted contents in neutrino mode are: $\nu_{\mu}-98.33 \%, \bar{\nu}_{\mu}-0.08 \%, \nu_{e}-1.56 \%, \bar{\nu}_{e} 0.03 \%$. The relative ratios of event-weighted contents in antineutrino mode are: $\nu_{\mu}-0.42 \%, \bar{\nu}_{\mu}-$ $98.07 \%, \nu_{e}-0.26 \%, \bar{\nu}_{e} 1.26 \%$.

### 3.3 Precision Measurement of the Flux from Events in the Detector

Precise knowledge of the neutrino flux is key to many of the physics goals of the experiment. The goal, which is ambitious, will be to measure the neutrino flux as a function of energy to a precision better than $0.5 \%$. This goal is a design-driver for the experiment. In this section, we outline an analysis plan to achieve this goal using the event types described in the previous section.

The flux will be determined through the following steps:

1. The inverse muon decay (IMD) events $\left(\nu_{\mu}+e^{-} \rightarrow \mu^{-}+\nu_{e}\right)$ are, in principle, ideal for measuring the total flux because the IMD cross section is well known in the Standard Model. Therefore, these events will be used to determine the normalization of the flux. An important background to this measurement, however, comes from the CCQE events ( $\nu_{\mu}+n \rightarrow \mu+p$ ), which must be subtracted. In this step, the predicted number of CCQE events is based on external cross section measurements. The error on the external cross section is likely to be the limiting systematic on the normalization determined in this step.
2. The shape of the flux is measured using the traditional "fixed $\nu$ " measurement method, which was applied in CCFR [85, 114]. and NuTeV [89], and is currently being used for in the Minos Experiment [131 to measure the shape of both the neutrino and antineutrino flux. The flux shape is then normalized by the IMD events from step 1 to obtain the initial flux prediction.
3. The initial flux prediction is used to determine a more precise CCQE cross section based on the NuSOnG data.
4. Step 1 is repeated using the more precise cross section determined in step 3 . This produces the final normalization which is used to scale the results of step 2, yielding the final flux.

When the analysis is performed, it may be more effective and efficient to combine the above steps into a single multiparameter fit to the IMD and CCQE data, constrained by the external cross section information. However, for transparency we will consider the stepwise approach below.

Reaching the goal of $\lesssim 0.5 \%$ systematic error depends mainly on the systematics of the IMD total event rate measurement. To set the scale of the problem, the best measurement of IMD events to date, from CHARM II, had a systematic error of $3 \%$ [132. Thus, we must achieve an order of magnitude improvement in the IMD total systematic error. While we present a well-grounded back-of-the-envelope argument below, this level of measurement has yet to be demonstrated by simulation. That is a priority for future work on the development of NuSOnG.


Figure 13: Momentum distribution of protons in $\nu$ CCQE events, from the Nuance Event generator.

Two useful cross checks of the measured NuSOnG flux are possible. First, one can extract an energy binned neutrino flux from the IMD events in step 1. Because of angular resolution, this flux may have substantial smearing, but it can be used as a compelling cross-check of the flux shape derived in step 2. Second, the neutrino to antineutrino flux ratio can be compared to the first principles prediction based on secondary production measurements.

### 3.3.1 Step 1: The IMD Measurement for Normalization

NuSOnG expects to observe > 200k IMD events during neutrino running. The high statistics is a consequence of both the high neutrino flux and high neutrino energy. High energy is required because the threshold for IMD scattering is $E_{\nu} \geq E_{\mu} \geq \frac{m_{\mu}^{2}}{2 m_{e}}=10.9$ GeV . The SSQT beam design for NuSOnG produces minimal flux below 30 GeV , well within the range of IMD production. This indicates that there will be high statistics for IMD events in all flux bins.

These events will be used for total flux normalization, with the shape determined using the Fixed $\nu$ method described in step 2. This is done because, while these events can in principle be fully reconstructed assuming that the incoming neutrino enters parallel to the z-axis, the reconstruction in practice suffers substantial smearing. At $\sim 100 \mathrm{GeV}$, IMD events will have scattering angles of $\lesssim 1 \mathrm{mrad}$. This is similar in magnitude to the expected divergence of the beam, which was 0.62 mrad in NuTeV . Angular resolution errors are expected to be at a similar level.

IMD events must be separated from background, mainly due to CCQE-like interac-
tions (which include both real CCQE interactions and single $\pi$ events where the pion was absorbed in the nucleus, and thus are effectively CCQE events). IMD events are qualitatively different from CCQE-like ones in two ways: there is no hadronic energy in the event, and there is a strict kinematic limit on the transverse momentum of the outgoing muon, $p_{T} \leq 2 m_{e} E_{\mu}$. It is therefore crucial to design NuSOnG for observation of very low hadronic energy in the presence of a muon track, and for excellent angular resolution on the outgoing muon. The fine segmentation of NuSOnG should allow hadron identification in the presence of a muon to substantially lower energy ( $\sim 0.75$ GeV ) compared to 1.5 GeV for Charm II [132] and 3 GeV for $\mathrm{NuTeV}[75]$. One can see from the momentum distribution of the protons produced in CCQE interactions, shown in Fig. 13, that this approach will allow NuSOnG to cut more of the CCQE background than was possible in the previous experiments. NuSOnG also expects better IMD resolution than Charm II, due to the finer segmentation, which will reduce backgrounds.

Events which produce very low energy pions can also produce a background, although at a lower level than the CCQE background. NuSOnG's open trigger will allow many of the low multiplicity DIS events and $\mathrm{CC} \pi^{+}$events to be identified and cut due to the presence of subsequent michel electrons which come from the $\pi^{+} \rightarrow \mu^{+} \rightarrow e^{+}$ decay chain. A 50 MeV michel electron will traverse 12 cm of glass, producing hits in up to four chambers in the vicinity of the interaction vertex.

The IMD method for determining the flux proceeds in the following manner. After cutting on hadronic energy, minimum energy for the outgoing muon, and no michel electrons near the vertex, the plot of muon $p_{T}$ will show a sharp peak at $p_{T} \sim 0$ superimposed on a broad continuum of background events extending to high $p_{T}$. The continuum is fit and extrapolated under the IMD peak, to extract the number of IMD events. This is divided by the theoretical cross section to yield the flux.

At the high energies of NuSOnG, the only nuclear effect expected for CCQE events comes from the Pauli exclusion effect. This produces an overall suppression of the cross section across all energies. Both the NuTeV and Charm II measurements suffered from the lack of availability of precise information on the Pauli exclusion effect. This resulted in an error on the Charm II measurement from the CCQE model of $2.1 \%$.

NuSOnG will be in the fortunate position that a number of new measurements of the CCQE cross section on nuclear targets will be available as inputs into the CCQE model. Results from MiniBooNE [133] and SciBooNE [134] will address Pauli suppression in CCQE interactions on carbon. Minerva [135] is studying a series of nuclear targets, and are willing to consider running a glass target for NuSOnG, if we were to supply the target panels. The precision on the CCQE cross section in the NuSOnG era may be $5 \%$, which is $\sim 5$ times better than the CHARM II era measurements. Thus, at this step, the CCQE model error for NuSOnG may be as low as $0.4 \%$.

A CCQE model error which was not addressed in the Charm II analysis was the long-standing discrepancy between models and data at low $Q^{2}$ 133. Low $Q^{2}$ events having small scattering angles represents a significant error on the extrapolation under the IMD peak. This discrepancy has recently been resolved by MiniBooNE under a dipole form-factor model [133]. Minerva plans to address the $Q^{2}$ dependence of the form factor in a model-independent way [136]. We will assume that the discrepancy will be fully addressed by the time of the NuSOnG run.

Another $1.5 \%$ systematic error in Charm II came from the model of the other sources
of low hadronic energy CC events, which are dominated by $\Delta$ resonant production. As described above, NuSOnG expects a substantially lower contamination from these sources because of the lower energy threshold and the michel electron veto. For those background events which are not cut, the modeling of these sources will substantially improved using Minerva data. In Minerva, the tracks from $\mathrm{CC} \pi^{+}$events are well reconstructed, so models $p_{T}$ distribution of outgoing muons can be tuned. Similarly, Minerva offers the opportunity to accurately parametrize CCpi ${ }^{0}$ events. Again, the total error on the low hadron multiplicity events in 2015 is expected to be on the order of $5 \%$, so the modeling of these backgrounds should not be a limiting systematic.

IMD events can be cut from the sample due to electromagnetic radiation of the muon near the vertex region which is mistakenly identified as hadronic energy at the vertex. The NuTeV IMD analysis [75] assigned a $1 \%$ systematic error due to radiative effects. We address this error in two ways. First, in the NuTeV experiment, the photons immediately converted in the 10 cm iron plates, while in NuSOnG, the 2.5 cm glass plates are $0.25 \lambda_{0}$, giving photons a $50 \%$ probability of traversing three plates before showering. Fewer IMD radiative events will therefore be misidentified as events with hadronic energy at the vertex. Second, because of the higher segmentation, NuSOnG will employ an improved model of electromagnetic showers, reducing the systematic error.

### 3.3.2 Step 2: The Fixed- $\nu$ Measurement to Determine the Shape

The central premise of the Fixed $\nu$ method for measuring the flux is that, for small hadronic energy exchange $(\nu)$, the differential cross section is independent of energy to a good approximation. The Fixed $-\nu$ method utilizes this fact to measure the relative flux between energy bins and the relative flux between neutrino and antineutrino interactions. External input is then needed to determine the overall normalization.

To motivate the premise, consider the differential cross section at a fixed $\nu$ integrated over all $x$ :

$$
\begin{equation*}
\frac{d \sigma}{d \nu}=A\left(1+\frac{B}{A} \frac{\nu}{E_{\nu}}-\frac{C}{A} \frac{\nu^{2}}{2 E_{\nu}^{2}}\right) . \tag{51}
\end{equation*}
$$

In this equation,

$$
\begin{align*}
A & =k \int F_{2}\left(x, Q^{2}\right) d x  \tag{52}\\
B & =-k \int\left[F_{2}\left(x, Q^{2}\right) \mp x F_{3}\left(x, Q^{2}\right)\right] d x  \tag{53}\\
C & =B-k \int F_{2}\left(x, Q^{2}\right)\left(\frac{\frac{1+2 M x}{\nu}}{1+R\left(x, Q^{2}\right)}-\frac{M x}{\nu}-1\right) d x, \tag{54}
\end{align*}
$$

where $k=\left(G_{F}^{2} M\right) / \pi$, and $\mp$ refers to neutrinos $(-)$ or antineutrinos $(+)$. For simplicity, first consider $\nu \rightarrow 0$. The cross section becomes equivalent to $A$, which is a constant. Since it is impossible to measure scattering for $\nu=0$, consider scattering for $\nu=\nu_{0}$ where $\nu_{0} \ll E_{\nu}$. As long as $\nu_{0}$ is small enough, the terms which depend on $\nu_{0} / E_{\nu}$ will have negligible contribution. Thus for a fixed, low value of $\nu, d \sigma / d \nu \rightarrow A$, independent of beam energy. Note that terms $B$ and $C$ differ for neutrinos and antineutrinos. However, as long as $\nu_{0} / E_{\nu}$ is negligible, these terms do not contribute and the cross section for antineutrinos is equal to the cross section for neutrinos.

From this, one can see how to measure the relative fluxes. If one measures the number of events at a given $\nu_{0}$ in bins of $E_{\nu}$, one can solve for the flux:

$$
\begin{equation*}
\Phi\left(E_{\nu}\right)=N\left(E_{\nu}, \nu_{0}\right) / A . \tag{56}
\end{equation*}
$$

The relative change of flux between two energy bins is independent of $A$ :

$$
\begin{equation*}
\Phi\left(E_{\nu}^{b i n 1}\right) / \Phi\left(E_{\nu}^{b i n 2}\right)=N^{b i n 1}\left(E_{\nu}, \nu_{0}\right) / N\left(E_{\nu}^{b i n 2}, \nu_{0}\right) \tag{57}
\end{equation*}
$$

Since the neutrino and antineutrino cross sections are equal, this method also allows the relative fluxes to be extracted, independent of $A$.

$$
\begin{equation*}
\Phi\left(E_{\nu}\right) / \Phi\left(E_{\bar{\nu}}\right)=N\left(E_{\nu}, \nu_{0}\right) / N\left(E_{\bar{\nu}}, \nu_{0}\right) \tag{58}
\end{equation*}
$$

Thus one can extract the relative bin-to-bin and neutrino-to-antineutrino fluxes strictly from the data, with no theoretical input on the value of $A$.

In practice one uses a low $\nu$ region, defined by $\nu<\nu_{0}$ where $\nu_{0}$ is some appropriate upper limit. CCFR and NuTeV, used $\nu<\nu_{0}=20 \mathrm{GeV}$, which allowed high statistical precision for the measurement. From the theoretical point of view, however, this was not optimal since the goal was to measure the flux down to $E_{\nu}=30 \mathrm{GeV}$, thus at $\nu=20 \mathrm{GeV}$, the $\nu / E_{\nu}$ terms were not negligible. The flux is then given by:

$$
\begin{equation*}
\Phi\left(E_{\nu}\right)=\int_{0}^{\nu_{0}} \frac{\frac{d N}{d \nu}}{1+\frac{B}{A} \frac{\nu}{E_{\nu}}-\frac{C}{A} \frac{\nu^{2}}{2 E_{\nu}^{2}}} d \nu . \tag{59}
\end{equation*}
$$

A fit to $d N / d \nu$ determines $B / A$ and $C / A$. One can test the quality of the bin-to-bin result by fitting $\sigma / E$ to a line. A good fit results in small slope, due to QCD effects on the order of a few percent (somewhat smaller in antineutrino mode), with small error. NuTeV found values consistent with expectation [89]:

$$
\begin{align*}
& \frac{\Delta\left(\frac{\sigma^{\nu}}{E}\right)}{\Delta E}=(-2.2 \pm 0.8) \% / 100 \mathrm{GeV}  \tag{60}\\
& \frac{\Delta\left(\frac{\sigma^{\bar{\nu}}}{E}\right)}{\Delta E}=(-0.2 \pm 0.8) \% / 100 \mathrm{GeV} \tag{61}
\end{align*}
$$

The NuTeV analysis indicated a good fit to a straight line, as expected. The extracted shape of the flux was obtained to very high precision across the full energy range by this approach.

NuSOnG has an important advantage over NuTeV when implementing this method, in that the high statistics and good segmentation will all us to reduce this range of the low $\nu$ substantially, perhaps to as low as $\nu<\nu_{0}=10 \mathrm{GeV}$. This should allow an even more precise measure of the shape than was obtained by past experiments, since the contribution of the fit to the $B$ and $C$ terms will be reduced. In particular, the systematic error contribution from the charm mass will be substantially reduced.

NuTeV also required $\nu>5 \mathrm{GeV}$ to cut the resonance region. NuSOnG is also likely to introduce such a cut. However, this should be revisited in light of the expected new data from Minerva in the resonance region.

The most important detector systematic to this measurement is likely to be the muon energy scale. NuTeV achieved knowledge of the muon energy scale to $0.7 \%$, although the absolute calibration beam was known to $0.3 \%$. The difficulty was mapping
across the full area of the toroids. For NuSOnG to achieve its goal of measuring the flux with $\lesssim 0.5 \%$ total error, the muon energy scale will need to be known to about $0.25 \%$. Careful thought must be put in to understand how to achieve this.

In past experiments, the next step was to obtain the absolute flux by normalizing to the world's total, which is $\sigma / E_{\nu}=0.667 \pm 0.014 \times 10^{-} 38 \mathrm{~cm}^{2} / \mathrm{GeV}$. It necessarily introduces a $2 \%$ normalization error into this method. NuSOnG will use the IMD events to perform the absolute normalization, rather than relying on the world average neutrino cross section measurement. This is done by scaling the total flux measured in neutrino mode with the Fixed $\nu$ method to $\sum_{i} N^{I M D}\left(E_{i}\right) \int \sigma^{I M D} d E$. At the end of this step, the predicted flux is expected to be known to $\sim 1 \%$.

### 3.3.3 Step 3: A Precise Measurement of the CCQE Cross Section

At this point in the procedure, the limiting systematic is likely to be the CCQE cross section model error in the IMD normalization. In this step, this cross section is further constrained using the CCQE data in NuSOnG.

The background to the CCQE cross section analysis will be the low hadronic energy events. These can be reduced using the michel veto method discussed in Step 1. Beyond this, because CCQE scatters extend to higher angles, excess hits due to the presence of charged pions and photons from $\pi^{0}$ decay should be more easily resolved from the photon track. NuSOnG expects $\sim 500 \mathrm{k}$ CCQE events, and thus stringent cuts can be applied to remove backgrounds without substantial statistical error, assuming the efficiency of the cuts can be well-understood.

The goal will be for NuSOnG to measure the CCQE cross section to $\lesssim 2 \%$. This would be a very valuable measurement in its own right, as well as allowing for improvement in the flux extraction in the following steps. This result can be used to constrain the normalization for a glass-target measurement in Minerva. Ratios to the other nuclear target cross section measurements by Minerva then allow precisely determined measurements at low E across a wide range of nuclei. This will be useful input to future precision neutrino oscillation measurements.

### 3.3.4 Step 4: The Final NuSOnG Flux

Once the CCQE cross section has been determined at the $\lesssim 2 \%$ level, one can iterate the IMD analysis of step 2 and then renormalize the distributions in step 3 . The resulting flux is expected to have errors of $\lesssim 0.5 \%$.

### 3.3.5 Cross Checks

Two useful cross checks of the flux are possible. The first takes the measured flux and compares it to the IMD event rate in energy bins. The second uses external data to cross check the shape and normalization of the antineutrino flux.

The first cross check compares the shape of the neutrino flux determined at step 1 to the shape determined through step 2. This will be done by running the final flux through the MC and using it to predict the IMD rate in energy bins. We will then extract the predicted flux in energy bins to compared to the measurement performed in step 1. This provides a powerful consistency check.

We can also cross check the fluxes obtained by the above method using a firstprinciples prediction based on external secondary production measurements. The absolute predictions in neutrino and antineutrino mode are unlikely to be an effective cross check because of large errors in the secondary production predictions, which vary from 5 to $10 \%$. However, the prediction of the ratio of the neutrino to antineutrino fluxes may be possible to high precision. This requires some investigation.

Reference [139] provides a compendium of secondary production experiments in Table 3. None extend up to 800 GeV . The most relevant experiment was NA56/SPY at 450 GeV , which took data on beryllium targets 70 . This experiment published yields of $\pi^{+}, \pi^{-}, K^{+}$and $K^{-}$with errors on each measurement of $\sim 5 \%$. However, because many of the systematics cancel in ratio, the $\pi^{-} / p i^{+}, K^{-} / K^{+}$and $\pi / K$ ratios are each determined to $\sim 2.5 \%$. This data should allow a good cross check of the individual $\pi$ and $K$ shape contributions. We may choose to run for a short period at 450 GeV in order to have an exact cross-comparison.

### 3.3.6 The Electron Neutrino Flux

We will begin by tuning the NuSOnG Beam Monte Carlo using the recent secondary meson production measurements described above. The new $K$ production results will improve the first principles prediction for electron neutrinos beyond those of NuTeV . The electron neutrino contamination then can be further constrained through the precision measurement of the $\nu_{\mu}$ flux, which can be tied to the $\nu_{e}$ flux, and through the measurement of $\nu_{e}$ CCQE events.

Once the muon neutrino flux is measured to high precision, it can be used to constrain the electron neutrino flux. This is because the $\nu_{e}\left(\bar{\nu}_{e}\right)$ background is largely due to $K^{+}\left(K^{-}\right)$decays in neutrino (antineutrino mode). Using the measured $\nu_{\mu}$ peak from $K^{+}$events, the beam Monte Carlo can be precisely tuned. Having measured the CCQE cross section precisely in the process of determining the $\nu_{\mu}$ flux, this result can then be applied to $\nu_{e}$ CCQE events to cross check the $\nu_{e}$ flux prediction.

## 4 Preliminary Design

This report focuses upon the determination of the physics goals of the experiment. In order to maintain realistic goals, we have developed a preliminary design for a beam and detector based on existing technology. There are two particularly challenging aspects of the design. The first is the high Tevatron intensity discussed in sec. 4.1. The second is the high precision required for the detector calibration discussed in sec. 4.3.3.

The 2007 Fermilab Steering Group Report considers the Tevatron-based neutrino beam described here. The preliminary concept for the facility recieved an endorsement [137.

### 4.1 Proton Delivery to NuSOnG

Our goal is to obtain $2 \times 10^{20}$ protons on target during a 5 -year run. This section outlines how we might achieve this goal.

Proton delivery occurs via the following lines:

- The Linac
- The Booster
- The Main Injector
- The Tevatron
- Extraction to targeting

The existing Linac and the Booster should perform to the level needed by NuSOnG without problems. The Booster fills the MI in batches of $5 \times 10^{12}$ protons and will operate between 9 and 15 Hz by 2015. The Proton Plan projects $7 \times 10^{13}$ protons in each MI fill by 2010 [138]. Two pulses from the MI are used to fill the Tevatron. In principle, therefore, it is conceivable that the Tevatron could receive nearly $1.5 \times 10^{14}$ protons per fill under this scenario.

Let's suppose that with care the Tevatron can accelerate $8 \times 10^{13}$ ppp to 800 GeV using two pulses from the Main Injector at $4 \times 10^{13}$ each pulse, similar to today's MI operation. To date, the highest intensities extracted from the Tevatron in a single pulse at 800 GeV were around 2.5 to $3 \times 10^{13}$. The limiting issue was longitudinal instabilities for energies above 600 GeV at high intensities, as the bunch length shrank. "Bunch spreaders" were used to compensate. A better method to compensate will be required for NuSOnG. However, advances in rf techniques and technology and in damper systems make finding a satisfactory solution conceivable. More detailed study is needed.

Our proposal is for a Tevatron cycle time of 40 s , with a 1 s flattop at 800 GeV . Since the MI cycle time will be 2.2 s , and we need two injections, our impact on NuMI is $4.4 / 40=11 \%$ of their run time.

If the uptime for the Tevatron is $66 \%$, then we will receive $5 \times 10^{5}$ cycles per year. At $8 \times 10^{13} \mathrm{ppp}$, this gives $4 \times 10^{19}$ protons per year. We then achieve our goal in five years of running.

### 4.2 Neutrino Beam Design

### 4.2.1 Target

Beryllium oxide was the target material in NuTeV and prior high energy neutrino beamlines [140, 141]. Beryllium is efficient at producing secondary mesons, and BeO has good structural and thermal properties. The NuTeV target consisted of two 30 cm long, 2.5 cm diameter segmented rods in a copper cooling block, mounted on a movable drive that could select between centering the beam on either of the two targets or no target. This target was designed to accept up to $1 \times 10^{13}$ protons per pulse (ppp). A similar target will be acceptable for NuSOnG, but it may be a challenge to provide adequate cooling at our design intensity of $8 \times 10^{13}$ protons per cycle. The NuTeV protons were delivered in five 4 msec "pings" separated by 0.5 sec ; we intend to have one pulse of about 200 msec . This means that our instantaneous heating rate will be somewhat lower than NuTeV's, but the total number of protons per cycle is eight times higher. In NuTeV the beam width was 0.6 mm , which was significantly smaller than necessary; a wider more diffuse beam would help relieve the localized heating problem. Careful design of the target support and cooling system will be a necessity.

### 4.2.2 SSQT

A Sign Selecting Quadrupole Train (SSQT) can be used to provide beams of either neutrinos or antineutrinos with very low contamination from either wrong-sign muon neutrinos or electron neutrinos from neutral kaons. The NuTeV SSQT utilized two dipoles and six quadrupoles, with two dumps [140, 141]. The first dipole provided a 6.1 mrad bend for 250 GeV daughter mesons of the selected sign. In antineutrino mode the unreacted protons are bent in the opposite direction and are absorbed in the first dump. In neutrino mode the protons are absorbed in the second dump. The first two quadrupoles capture the secondary beam. A second dipole then bends the beam by another 1.6 mrad , enhancing the sign separation and sweeping out low energy particles produced by scraping in upstream magnets. Neutral particles are not bent and therefore travel away from the detector. NuSOnG will use a similar SSQT. The only challenge will be designing the proton dumps for our significantly higher intensity. In the NuTeV upstream dump in antineutrino mode, the dump temperature approached 100 C at $1.3 \times 10^{13}$ protons per pulse; the temperature limit was 110 C . The NuSOnG dumps will need to be water-cooled.

### 4.2.3 Monitoring

Primary beam monitoring in NuTeV was accomplished with four beam position monitors (BPMs), four vacuum segmented wire ionization chambers (SWICs), four secondary emission electron detectors (SEEDs), a beam current toroid, and a thin foil secondary emission monitor (SEM) [140, 141. The toroid, SEM, SEEDs and BPMs measured proton intensity; the BPMs, SWICs, and SEEDs monitored position. It was found that the SEM degraded over the course of the run, so the beam toroid was used as the primary measure of intensity. The BPMs and SEEDs gave closely correllated position measurements, and the SWICs and SEEDs gave beam profiles that agreed well except in the tails; the SEED tails dropped more rapidly than those from the SWICs. With the exception of the SEMs, which would suffer even more radiation damage at

| Parameter | Value |
| :--- | ---: |
| Total target mass | 3.492 |
| Fiducial mass | 2.975 kt |
| Total length | 192 m |
| Number of glass planes | 2500 |
| Number of toroid washers | 96 |
| Number of muon detector wire planes | 60 |
| (two coordinates each) |  |

Table 3: Summary of NuSOnG detector parameters.
our higher intensities, a combination of any of these monitoring devices could be used by NuSOnG.

### 4.3 Detector Design

This section details our first ideas about the detector configuration; these are summarized in Tab. 3. In thinking about NuSOnG, we have drawn on previous large, high energy neutrino detectors whose characteristics are summarized in Table 4 . NuSOnG represents a natural evolution of these designs and we believe this makes construction low risk. Of particular note regarding Table 4 is the excellent performance achieved by CHARM II using digital proportional tubes, a glass target, and fine granularity.

The primary event signatures NuSOnG will need to identify are:

- charged current deep inelastic scattering, characterized by a hadronic shower and a high energy muon
- neutral current deep inelastic scattering, characterized by a hadronic shower
- inverse muon decay, $\nu_{\mu}+e^{-} \rightarrow \mu^{-}+\bar{\nu}_{e}$, which is characterized by a high energy muon accompanied by no hadronic activity.
- neutrino and antineutrino electron scattering, characterized by an electromagnetic shower with no hadronic activity
- stopped muon decay, which results in an electromagnetic shower with energy up to 50 MeV . These events will be used to reject low hadronic energy events which are tagged through the $\pi \rightarrow \mu \rightarrow e$ decay chain (see sec. 3.3.1).
In order to achieve the rates and carry out the measurements given in Section 3, NuSOnG consists of a 3.5 kton ( 3 kton fiducial volume) isoscalar target with high segmentation resulting in good separation between electromagnetic and hadronic showers and muon tracks with good energy resolution for each. Good separation between hadronic and electromagnetic showers and good muon identification are necessary for separation of neutral and charged current events, and for low systematic errors on the measurements of the neutrino and antineutrino electron scattering cross sections. Finally, good muon identification is critical for detecting inverse muon decay events for a precise flux measurement.

Given the large size of the detector, ease of construction and low cost technologies are important. The long running time requires high stability and robust operation.

|  | EM | Resolution <br> Hadronic <br> $\left(\sigma_{E} / E\right)$ | Muon <br> $\left(\sigma_{p} / p\right)$ | Sampling | Absorber |
| :--- | :---: | :---: | :---: | :---: | :---: |
|  | $1.04 / \sqrt{E}$ | $0.72 / \sqrt{E}$ | $8 \%$ | $0.11 \mathrm{X}_{o}$ | sand/shot |
| FMMF <br> (Flash tubes, <br> digital) |  |  | $5 \%$ | $2.8 / 8.3 \mathrm{X}_{o}$ | steel |
| CDHS | $0.80 / \sqrt{E}$ | - | $5 \%$ | $0.5 \mathrm{X}_{o}$ | glass |
| (Scintillator) <br> CHARM II <br> (Prop. tubes, <br> digital) | $0.52 / \sqrt{E}+0.02$ | $0.24 / \sqrt{E}+0.34$ | $5 \%$ |  |  |
| NuTeV <br> (Scintillator) | $0.86 / \sqrt{E}+0.022$ | $0.5 / \sqrt{E}+0.042$ | $10 \%$ | $5.8 \mathrm{X}_{o}$ | steel |

Table 4: Comparison of high energy neutrino detectors.

Our first design is shown in Figs. 14 and 15 and summarized in Table 3. NuSOnG consists of four calorimeters each with a muon spectrometer. 15 m decay volumes separate the four detector elements. Interspersing the decay volumes between the detectors will allow a calibration beam to be brought to each of the four detector regions.

Each calorimeter has $500 \mathrm{SiO}_{2} 2.5 \mathrm{~cm}\left(\mathrm{X}_{o} / 4\right)$ glass target planes interleaved with active detectors with two dimensional readout. The active detectors could be proportional tubes, scintillator panels, or a combination of both. These three options are discussed below. Neutrinos interact in the target planes, creating secondary particles; the active detector determines the total energies of the hadronic and electromagnetic secondaries. The muon detector measures the momentum of muon secondaries and serves to identify them. The pattern of the shower serves to identify the shower type: showers in which all the energy resides in ten of fifteen planes will be electromagnetic, and more extended showers will be hadronic. The lateral extent of the shower also resolves electromagnetic from hadronic showers.

We have chosen an $\mathrm{SiO}_{2}$ target. This material provides a balance between longer radiation length, important to particle ID issues, and shorter detector length, important for acceptance and calibration issues. The target could be commercial glass or thin walled plastic boxes filled with sand. Glass planes have the advantage of being easy to install and require no construction. Sand-filled boxes could be much less expensive. We will investigate both possibilities. Either way, $\mathrm{SiO}_{2}$ has the advantage of being isoscalar $\left(\left\langle N_{u}\right\rangle>/\left\langle N_{d}\right\rangle=0.998\right)$. $\mathrm{SiO}_{2}$ has a density of $2.2 \mathrm{~g} / \mathrm{cm}^{3}$; a high energy muon will lose 10 MeV per plane, which gives 5 GeV across all 500 planes in one calorimeter. Energy loss will also occur through electromagnetic showers. An example straightthrough muon event from our initial GEANT4 detector simulation is shown in Fig. 16 . A michel electron with 30 MeV energy should be clearly visible across three planes. Each calorimeter is followed by a toroidal muon spectrometer consisting of magnetized iron plates interleaved with drift chambers.

Other target materials, including emulsion, are under consideration, as has been discussed in previous sections of this document. These materials are not yet incor-


Figure 14: NuSOnG detector showing calorimeter modules and muon detector.


Figure 15: The full NuSOnG experiment showing four detectors separated by a decay volume.


Figure 16: A 100 GeV muon traversing the detector from the NuSOnG initial GEANT4 Monte Carlo.
porated into the preliminary design presented here, but should be straightforward to include in the future.

The design must address beam correlated backgrounds. These include backgrounds arising from debris (muons, remnants of hadronic showers) from neutrino interactions in the earth surrounding the detector. We plan for a forward veto consisting of a three layer scintillator hodoscope. Since our detector is so long, we may also need a veto system along the sides, top, and bottom of the calorimeters. We plan a Monte Carlo study of veto requirements in the coming months. Cosmic rays muons and their attendant showers present a beam-uncorrelated background which we will need to eliminate. We envisage a counter on the top of the detector similar to that used by the MINOS experiment.

NuTeV showed the value of continuous beam calibration and this will be discussed in a separate section.

While our detector is quite large, the robust, simple design will make the cost and construction manageable. The modules design makes upgrades and improvements straightforward. While we are designing with an initial four to five year run in mind, this detector can be put to other uses should the physics warrant.

### 4.3.1 Active detector options

The active detector performs two roles: first, it tracks the particles emerging from a neutrino interaction; second, it samples the particle's energy loss along the trajectory giving an measurement of the total energy. Simplicity, robustness, and high efficiency are essential, as is low cost.

Two technologies immediately present themselves: gas-filled proportional tubes and plastic scintillator read out by phototubes. Both have been used in several experiments (see Table 4). At this point, it is not clear to us which is the best approach for NuSOnG. We are also considering a design with both proportional tubes and scintillator. In the coming months, we plan to study the performance of each via simulation, develop preliminary design prototypes, and carry out a detailed cost estimate. We describe each detector concept below.

### 4.3.1.1 Proportional Tubes

A first design for a proportional tube active detector is shown in Fig. 17. Each active detector plane is made from five $1 \mathrm{~m} \times 5 \mathrm{~m}$ extruded aluminum panels. Each panel contains fifty $1 \mathrm{~cm} \times 2 \mathrm{~cm}$ drift cells. A $50 \mu \mathrm{~m}$ wire is strung down the center of each tube, and the applied high voltage produces both drift and proportional amplification fields. Ar: $\mathrm{CO}_{2}$ (80:20) provides a good candidate for a fill gas; with $1.8-2 \mathrm{kV}$ applied to the wire, the drift field will give a drift velocity of about $50 \mu \mathrm{~m} / \mathrm{ns}$ and a gain of 3000. A minimum ionizing particle crossing the 1 cm cell will deposit 2.7 keV of energy, liberating about 160 drift electrons in ten or so clusters. The drift time across the cell will be about 500 ns and proportional multiplication will give a collected charge of 80 fC over a time of 250 ns .

As an example of a readout scheme, we look to the ATLAS Transition Radiation Tracker (TRT) ASIC chips. The TRT readout has a peaking time of 7.5 ns and a charge threshold of 2 fC , making them well matched to our proportional tubes. Each chip set reads out sixteen channels and can be configured to provide trigger information.


Figure 17: Proportional tubes design.

The TRT system, which is based around 6 mm straw tubes, has achieved a spatial resolution of $127 \mu \mathrm{~m}$, albeit with higher energy deposition resulting from the use of a xenon mixture. Scaling by the energy deposition gives a resolution of $200 \mu \mathrm{~m}$ for our argon-filled tubes. The TRT readout chip set has sufficient charge sensitivity to allow us to use charge division; this should give position resolution of $5-10 \mathrm{~cm}$ along the wire.

### 4.3.1.2 Scintillating Strips

The second option uses planes of scintillator strips read out with green wavelengthshifting fibers fed into multi-anode photomultipliers. This option would be similar to that used for the SciBar detector in K2K, the Minos neutrino detector, and the Opera neutrino detector. NuSOnG would have 25005 m by 5 m planes with each plane made up of $1283.9 \mathrm{~cm} \times 1.3 \mathrm{~cm}$ strips. Each 64 strip plane will be separately wrapped in an Al skin that will provide the light seal and strength for the module.

The scintillator strips will be coextruded with a $\mathrm{TiO}_{2}$ reflective coating and have a 1.8 mm diameter hole in the middle. A 1.5 mm diameter green wavelength-shifting fiber will be put in the hole and routed to multianode photomultipliers for readout. The 64
wavelength-shifting fibers on one side of a plane will be coupled to a Hamamatsu M64 multianode photomultiplier tube. The readout side will alternate between subsequent planes to improve uniformity. The fiber end opposite to the tubes will be polished and mirrored to increase the light output and uniformity. Planes will alternate between horizontal and vertical strips to provide two view tracking; readout tubes will alternate.

The readout would be based on a custom ASIC combined with a standard FPGA. One example is the 64 channel MAROC2 custom integrated circuit, designed at LAL (Orsay) for the ATLAS luminosity monitor. This chip allows adjustment of the electronic gain of each of the 64 channels, which will be needed to correct for the expected factor of 3 pixel-to-pixel gain variation of the M64 tubes. The system provides a selftriggering analog readout into an external flash ADC. A fast discriminator signal for triggering is also available for each strip with a common threshold.

Based on the performance of the SciBar detector, a minimum ionizing particle traversing a strip will yields about 20 photoelectons close to the tube, and the strip/fiber system will have an attenuation length of 3.5 m . This would then produce about 10 photoelectrons at the center of the detector per plane.

### 4.3.1.3 Hybrid Design

Our initial estimates indicate the scintillator option may cost more than the proportional tube option. However, the scintillator system described above does provide a stable, easy to characterize active detector. In particular, scintillating strips offer very stable response that does not vary with pressure or temperature. We will investigate a hybrid system in which every fourth or eighth plane (one or two radiation lengths) would be a scintillator panel. The high granularity of the proportional tube design would give good pattern recognition, and the excellent energy resolution of the scintillator would give a better energy measurement. Reducing the fiber spacing in the scintillator may be possible; this would reduce the cost.

One issue with adding $12-25 \%$ scintillator would be the change in the fraction of protons in the detector. The precise change depends on the scintillator used, but for $\mathrm{CH}_{4}$ and one scintillator panel every quarter radiation length, the proton-neutron ratio changes from 0.998 to 0.940 . The impact of this change will have to be balanced against the cost reduction and stability improvement. This will be part of our Monte Carlo effort in the coming months.

### 4.3.2 Toroid Spectrometers

High energy muons produced in charged-current interactions will be momentum analyzed in three iron toroid spectrometers downstream of each subdetector (set of ten "stacks"). Each spectrometer will be composed of layers of magnetized iron instrumented with drift chambers for tracking.

Since NuSOnG will see muons of the same energies as NuTeV/CCFR a similar arrangement for measuring muon momenta would be suitable. CCFR used sections of 8 " thick steel washers instrumented with scintillator hodoscopes for calorimeter ${ }^{2}$

[^291]

Figure 18: Conceptual Schematic for a NuSOnG toroid element. The three sections contain the same amount of steel (eight washers of 8 " each). The upstream most section has additional drift chamber stations to improve acceptance for low energy muons. Each of the five drift chamber stations has 3 x and 3y view chambers.

Tracking was performed using four views of each x and y chambers ( 0.5 mm coordinate resolution) in three gaps located after each 1.6 m of steel. The magnetic field was produced by four coils carrying approximately 1500 A each which passed through the center hole. The field was nearly radially symmetric and pointed in the azimuthal direction with magnitude ranging from 1.9 T near the center hole to 1.55 T near the outer edge (at $\mathrm{R}=1.8 \mathrm{~m}$ ). Details can be found in reference [142].

Figure 18 shows a possible arrangement for a NuSOnG toroid spectrometer. One "Upstream section" and two downstream "Standard sections" are shown. The downstream sections contain eight 8 " washers with one drift chamber station with 3 x and $3 y$ view chambers each. The most upstream section of a spectrometer unit has two additional drift chamber stations to improve acceptance for low energy muons. To pass the coil through this arrangement the upstream chamber stations would be half size (the same chambers but rotated for each view). Each of the three sections contain the same amount of steel. Hodoscope paddles could be added in each chamber station for triggering purposes. Resolution of this arrangement would be dominated by multiple Coulomb scattering and would be $\sim 11 \%$ independent of momentum.

The NuSOnG arrangement will provide good acceptance for high energy primary muons of both signs since in a sign-selected beam the can be routinely operated with the polarity set to focus the primary muon. Very high energy particles can be tracked into the downstream target sections with a long lever arm and their momentum analyzed. (resolution for very high energy muons ( $>150 \mathrm{GeV}$ was limited in NuTeV and CCFR; this resulted in large uncertainties in measuring flux in the high energy tail of the beam). Improving flux measurements in this region may help constrain kaon fluxes and therefore electron neutrino beam contamination.

### 4.3.3 Detector Calibration

A thorough and precise calibration of the entire detector will be required to achieve the physics goals of NuSOnG. Some of the response features of the detector can be understood using beam and cosmic ray muon samples, but a dedicated calibration effort will be required to study the hadronic and electromagnetic response of the detector and to measure the absolute energy scales. Precise calibration of a detector of this size will require a dedicated in situ calibration beam such as was used in NuTeV for this purpose [143].

The requirements for NuSOnG calibration beam would be similar to those of NuTeV. Tagged beams of hadrons, electrons, and muons over a wide energy range $(5-200 \mathrm{GeV})$ would be required. The calibration beam should have the ability to be steered over the transverse face of the detector in order to map the magnetic field of each toroid with muons. This could be accomplished in several ways; for example, gaps of a few meters in front of each toroid could be incorporated into the design, and the beam could be steered into each toroid in turn; or the toroids could each be moved into the test beam for these calibration runs. Steering for hadrons and electrons would be less crucial than it was in NuTeV's case but would still be useful.

The calibration beam can be constructed with a similar design to NuTeV. Upstream elements were used to select hadrons, electrons, or muons. An enhanced beam of electrons was produced by introducing a thin lead radiator into the beam and detuning the portion of the beam downstream of the radiator. A radiator was also used in the nominal beam tune to remove electrons. Particle ID (a threshold cerenkov and TRDs) was incorporated in the spectrometer and used to tag electrons when running at low energy. A pure muon beam was produced by introducing a 7 m long beryllium filter in the beam as an absorber.

The NuTeV calibration spectrometer was able to determine incoming particle momenta with a precision of better than $0.3 \%$ absolute. This was accomplished by two means. First, precisely calibrated dipole spectrometer magnets were used, with $\int B d \ell$ known to better than $0.1 \%$ in the region traversed by the beam. Secondly, the bend angle was determined to better than $0.1 \%$ using drift chambers positioned over the 150 m spectrometer. This long lever arm allowed a modest alignment uncertainty of a few mm to translate into only a $0.1 \%$ uncertainty in the absolute momentum scale. The event-by-event resolution of the spectrometer, dominated by multiple scattering in the drift chamber walls, was better than $0.3 \%$ for most energies. (Helium in the region between the last dipole and the upstream part of the detector reduced the scattering in air).

Figure 19 shows the NuTeV calibration beam configuration and the long lever arm spectrometer used to tag particle momenta with an absolute precision of better than $0.3 \%$. The most downstream dipole was mounted on a rotating stand which gave the ability to steer the beam out of the plane.

The NuSOnG goal of the calibration precision would be to measure energy scales to a precision of about $0.5 \%$. NuTeV achieved $0.43 \%$ precision on absolute hadronic energy scale and $0.7 \%$ on absolute muon energy scale (dominated by the ability to accurately determine the toroid map). Precise knowledge of the muon energy scale is especially important in order to achieve high measurement accuracy on the neutrino fluxes using the low- $\nu$ method. For example a $0.5 \%$ precision on muon energy scale translates into about a $1 \%$ precision on the flux. Both energy scales are important




Figure 19: (Top) Components of the NTEST beamline used to calibrate the NuTeV detector. Four different thicknesses of converter material at NTACON were used to select pure hadrons or electrons. The 7 m long Be filter(NTBBE) was used to select pure muons. The numbers on the left-hand-side of each component indicate the relative distance of the component to the primary target (NT8TGT) in meters. (Bottom) NuTeV's long lever arm spectrometer. The four dipole bend magnets were located in an enclosure approximately 70 m upstream of the Lab E detector. The spectrometer spanned over 150 m in length; this allowed precision measurement of the bending angle.
for precision structure function measurements and were the largest contributions to structure function measurement uncertainties in NuTeV 89 .

### 4.4 Possible Locations

Fig. 20 shows a possible location for the NuSOnG beam target hall and detector. Other layouts are possible; this is just meant to provide an example.

This layout assumes that the beam is extracted at A0 from the TeVatron and directed through the Switchyard Complex to a new targeting hall. This location allows low luminosity extraction down existing beamlines for the calibration beam.

The detector is located near the New Muon Lab. This is a region with more than 200 m of clear length, with roads and utilities nearby.

The calibration beam could be delivered to the NuSOnG hall using a scheme similar to that used in NuTeV with the NTest beamline. Only a short extension of the existing NTest line would be required to reach a detector located near the New Muon Lab. The beam was split off from the same beamline (Ncenter) and then bent around to impinge on the detector at a 43 mrad angle.


Figure 20: Aerial view of Fermilab showing the Tevatron, external beam lines and potential site for NuSOnG target and detector halls.

## 5 Summary

NuSOnG is an experimental program with high discovery potential. The precision neutrino scattering measurements probe terascale physics and will complement discoveries at the LHC. Through precision electroweak measurements, NuSOnG will be sensitive to such new phenomena as extra $Z$ bosons with masses beyond the 1 TeV (depending on the model) and compositeness scales above 5 TeV . The NuSOnG measurement of the coupling to the $Z$, when combined with the LEP measurement of the invisible width, is a more sensitive method to search for new physics than this same measurement at the ILC. NuSOnG can also probe the existence of neutrissimos, moderately heavy neutral heavy leptons which may be produced at the LHC, but which could be difficult to reconstruct and identify. A wide range of direct searches for new particles and interactions can be accomplished. The high neutrino flux and isoscalar target will make allow measurements which probe deeper into nuclear structure.

The high energy neutrino facility, which uses 800 GeV protons from the TeVatron, has been endorsed by the 2007 Fermilab Steering Group. While NuSOnG is the first to propose an experiment for this facility, a wide range of interesting measurements can be made on this line.

The proposed 3 kton (fiducial) NuSOnG detector design, which is opitmized for the physics goals, is based largely on the experiences of NuTeV and CHARM II. The basic technology is straightforward, although challenges exist because of the high precision demanded by the physics goals. Detailed simulations of the detector are now underway

Our plan is to develop these ideas over the coming months. We plan to submit a proposal to the Fermilab Directorate in the near future.

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# QCD PRECISION MEASUREMENTS AND STRUCTURE FUNCTION EXTRACTION AT A HIGH STATISTICS，HIGH ENERGY NEUTRINO SCATTERING EXPERIMENT：NuSOnG 

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We extend the physics case for a new high－energy，ultra－high statistics neutrino scat－ tering experiment，NuSOnG（Neutrino Scattering On Glass）to address a variety of issues including precision QCD measurements，extraction of structure functions，and the derived Parton Distribution Functions（PDF＇s）．This experiment uses a Tevatron－based neutrino beam to obtain a sample of Deep Inelastic Scattering（DIS）events which is over two orders of magnitude larger than past samples．We outline an innovative method for


#### Abstract

fitting the structure functions using a parametrized energy shift which yields reduced systematic uncertainties. High statistics measurements, in combination with improved systematics, will enable NuSOnG to perform discerning tests of fundamental Standard Model parameters as we search for deviations which may hint of "Beyond the Standard Model" physics.


Keywords: Neutrino scattering on glass.

## 1. Introduction

### 1.1. NuSOnG: Precision structure functions and incisive QCD measurements

The search for new physics at the "Terascale" - energy scales of $\sim 1 \mathrm{TeV}$ and beyond - is the highest priority for particle physics. NuSOnG is a proposed high energy, high statistics neutrino scattering experiment that can search for "new physics" from the keV through TeV energy scales via precision electroweak and QCD measurements. During its five-year data acquisition period, the NuSOnG experiment could record almost one hundred thousand neutrino-electron elastic scatters, and hundreds of millions of Deep Inelastic Scattering (DIS) events, exceeding the current world data sample by more than an order of magnitude. This experiment can address concerns related to extraction of structure functions and their derived Parton Distribution Functions (PDF's), investigate nuclear corrections, constrain isospin violation limits, and perform incisive measurement of heavy quarks.

For example, with its high intensity sign-selected $\nu$ and $\bar{\nu}$ beams, NuSOnG can generate a very large ( $\sim 600$ million event) DIS sample. This extraordinary sample can be used to measure up to six structure functions (three on neutrinos and three on antineutrinos), which in turn provide knowledge of the PDF's which describe the momentum distribution of quarks as a function of $Q^{2}$. These measurements influence a variety of topics including nuclear effects and isospin violation.

NuSOnG is particularly well suited to study both the strange and antistrange PDF's using the sign-selected beam. The strange PDF's provide the input to the Paschos-Wolfenstein (PW) ${ }^{1}$ style analysis from which the electroweak parameters are extracted; NuSOnG should have sufficient data to do a fully self-consistent analysis. ${ }^{\text {a }}$

NuSOnG can also generate a wealth of neutrino elastic scattering (ES) and quasielastic scattering, including Inverse Muon Decay (IMD) events which would also provide unparalleled precision measurements. In particular, the ES measurement is a theoretically robust, purely leptonic measurement, hence this quantity is well suited for incisive Standard Model tests.

In the present paper, we discuss those aspects of NuSOnG that impact the QCD measurements, both directly and indirectly; this includes the extraction of

[^292]Table 1. Comparison of statistics and targets for parton distribution studies in NuSOnG compared to the two past highest statistics DIS neutrino scattering experiments.

| Experiment | $\nu$ DIS <br> events | $\bar{\nu}$ DIS <br> events | Main <br> target | Isoscalar <br> correction |
| :---: | :---: | :---: | :---: | :---: |
| CCFR | 0.95 M | 0.17 M | iron | $5.67 \%$ (Ref. 4) |
| NuTeV | 0.86 M | 0.24 M | iron | $5.74 \%$ (Ref. 5) |
| NuSOnG | 606 M | 34 M | glass | isoscalar |

the structure functions and the resulting PDF's, associated nuclear effects, isospin (charge symmetry) violation, and heavy quark issues. The purely electroweak measurements have been addressed in a separate publication. ${ }^{3}$ The combined set of NuSOnG measurement provides a rich multifaceted program for performing precision measurements and searching for new phenomena at energies ranging from the keV to TeV scales.

## 2. Deep Inelastic Scattering and Parton Distribution Functions

Obtaining a high quality model of the parton distribution functions in neutrino and antineutrino scattering is crucial to the NuSOnG electroweak measurements. ${ }^{3}$ NuSOnG will go a step beyond past experiments in addressing the systematics of PDF's by making high statistics measurements for neutrino and antineutrino data separately. Table 1 shows the large improvement in statistics for NuSOnG compared to NuTeV and CCFR, the previous highest statistics experiments. Issues of uncertainties on the nuclear corrections are avoided by extracting PDF's on $\mathrm{SiO}_{2}$ directly, in similar fashion to the NuTeV PW analysis.

The differential cross-sections for neutrino and antineutrino CC DIS each depend on three structure functions: $F_{2}, x F_{3}$ and $R_{L}$. They are given by

$$
\begin{align*}
\frac{d^{2} \sigma^{\nu(\bar{\nu}) N}}{d x d y}= & \frac{G_{F}^{2} M E_{\nu}}{\pi\left(1+Q^{2} / M_{W}^{2}\right)^{2}} \\
& \times\left[F_{2}^{\nu(\bar{\nu}) N}\left(x, Q^{2}\right)\left(\frac{y^{2}+(2 M x y / Q)^{2}}{2+2 R_{L}^{\nu(\bar{\nu}) N}\left(x, Q^{2}\right)}+1-y-\frac{M x y}{2 E_{\nu}}\right)\right. \\
& \left. \pm x F_{3}^{\nu(\bar{\nu}) N} y\left(1-\frac{y}{2}\right)\right] \tag{1}
\end{align*}
$$

where $+(-)$ is for $\nu(\bar{\nu})$ scattering. In this equation, $x$ is the Bjorken scaling variable, $y$ the inelasticity, and $Q^{2}$ the squared four-momentum transfer. The structure functions are directly related to the PDF's.

The function $x F_{3}\left(x, Q^{2}\right)$ is unique to the DIS cross-section for the weak interaction. It originates from the parity-violating term in the product of the leptonic
and hadronic tensors. For an isoscalar target, in the quark-parton model, where $s=\bar{s}$ and $c=\bar{c}$,

$$
\begin{align*}
& x F_{3}^{\nu N}(x)=x(u(x)+d(x)+2 s(x)-\bar{u}(x)-\bar{d}(x)-2 \bar{c}(x)),  \tag{2}\\
& x F_{3}^{\bar{\nu} N}(x)=x F_{3}^{\nu N}(x)-4 x(s(x)-c(x)) \tag{3}
\end{align*}
$$

In past experiments, the average of $x F_{3}$ for neutrinos and antineutrinos has been measured. Defining $x F_{3}=\frac{1}{2}\left(x F_{3}^{\nu N}+x F_{3}^{\bar{\nu} N}\right)$, at leading order in QCD,

$$
\begin{equation*}
x F_{3, \mathrm{LO}}=\sum_{i=u, d \cdots} x q_{i}\left(x, Q^{2}\right)-x \overline{q_{i}}\left(x, Q^{2}\right) . \tag{4}
\end{equation*}
$$

To the level that the sea quark distributions have the same $x$ dependence, and thus cancel, $x F_{3}$ can be thought of as probing the valence quark distributions. The difference between the neutrino and antineutrino parity violating structure functions, $\Delta\left(x F_{3}\right)=x F_{3}^{\nu N}-x F_{3}^{\bar{\nu} N}$, probes the strange and charm seas (cf. Sec. 6).

The function $F_{2}\left(x, Q^{2}\right)$ appears in both the cross-section for charged lepton ( $e$ or $\mu$ ) DIS and the cross-section for $\nu$ DIS. At leading order,

$$
\begin{equation*}
F_{2, \mathrm{LO}}=\sum_{i=u, d \cdots} e_{i}^{2}\left(x q_{i}\left(x, Q^{2}\right)+x \overline{q_{i}}\left(x, Q^{2}\right)\right), \tag{5}
\end{equation*}
$$

where $e_{i}$ is the charge associated with the interaction. In the weak interaction, this charge is unity. For charged-lepton scattering mediated by a virtual photon, $e_{i}$ is the fractional electromagnetic charge of the quark flavor. Thus $F_{2}^{\nu N}$ and $F_{2}^{e(\mu) N}$ are analogous but not identical and comparison yields useful information about specific parton distribution flavors ${ }^{6}$ and charge symmetry violation as discussed below. In past neutrino experiments, $F_{2}^{\nu}$ and $F_{2}^{\bar{\nu}}$ have been taken to be identical and an average $F_{2}$ has been extracted, although this is not necessarily true in nuclear targets, as discussed below.

Similarly, $R_{L}\left(x, Q^{2}\right)$, the longitudinal to transverse virtual boson absorption cross-section ratio, appears in both the charged-lepton and neutrino scattering cross-sections. To extract $R_{L}$ from the cross-section, one must bin in the variables $x, Q^{2}$ and $y$. This requires a very large data set. To date, the best measurements for $R_{L}$ come from charged lepton scattering rather than neutrino scattering. ${ }^{7}$ Therefore, neutrino experiments have used charged lepton fits to $R_{L}$ as an input to the measurements of $x F_{3}$ and $F_{2} .{ }^{8}$ This, however, is just a matter of the statistics needed for a global fit to all of the unknown structure functions in $x$ and $Q^{2}$ bins. ${ }^{9}$ With the high statistics of NuSOnG, precise measurement of $R_{L}$ will be possible from neutrino scattering for the first time.

As an improvement on past experiments, the high statistics of NuSOnG allows measurement of up to six structure functions: $F_{2}^{\nu}, F_{2}^{\bar{\nu}}, x F_{3}^{\nu}, x F_{3}^{\bar{\nu}}, R_{L}^{\nu}$ and $R_{L}^{\bar{\nu}}$. This is done by fitting the neutrino and antineutrino data separately in $x, y$ and $Q^{2}$ as described in Eq. (1). The first steps toward fitting all six structure functions independently were made by the CCFR experiment, ${ }^{10}$ however statistics were such that only $x F_{3}^{\nu}, x F_{3}^{\bar{\nu}}$, and $F_{2}$-average and $R$-average could be measured, where the
average is over $\nu$ and $\bar{\nu}$. A global fit of up to six structure functions in NuSOnG would allow separate parametrizations of the underlying PDF's which can account for the nuclear and isospin violation issues discussed below.

In addition to fitting to the inclusive DIS sample, neutrino scattering can also probe parton distributions through exclusive samples. A unique and important case is the measurement of the strange sea through charged current (CC) opposite sign dimuon production. When the neutrino interacts with an $s$ or $d$ quark, it can produce a charm quark that fragments into a charmed hadron. The charmed hadron's semileptonic decay (with branching ratio $B_{c} \sim 10 \%$ ) produces a second muon of opposite sign from the first:

$$
\begin{align*}
\nu_{\mu}+N \rightarrow \mu^{-}+ & c+X \\
& \hookrightarrow s+\mu^{+}+\nu_{\mu} . \tag{6}
\end{align*}
$$

Similarly, with antineutrinos, the interaction is with an $\bar{s}$ or $\bar{d}$,

$$
\begin{align*}
\bar{\nu}_{\mu}+N \rightarrow \mu^{+}+ & \bar{c}+X \\
& \hookrightarrow \bar{s}+\mu^{-}+\bar{\nu}_{\mu} . \tag{7}
\end{align*}
$$

The opposite sign of the two muons can be determined for those events where both muons reach the toroid spectrometer. Study of these events as a function of the kinematic variables allows extraction of the strange sea, the charm quark mass, the charmed particle branching ratio $\left(B_{c}\right)$, and the Cabibbo-Kobayashi-Maskaka matrix element, $\left|V_{c d}\right|$.

## 3. Experimental Extraction of Structure Functions in NuSOnG

### 3.1. Description of NuSOnG

The NuSOnG detector was designed to be sensitive to a wide range of neutrino interactions from $\nu$-electron scattering as well as $\nu$-nucleon scattering, though this paper focuses mainly on the latter process. The design has been described in detail in Refs. 3 and 11 and so we provide only a brief summary here.

The neutrino beam would be produced via a high energy external proton beam from a high intensity accelerator with energy of $\sim 1 \mathrm{TeV}$. The Fermilab Tevatron is an existing example. The CERN SPS,$+{ }^{12,13}$ which is presently under consideration because of its value to the LHC energy and luminosity upgrades and to a future beta beam, is a second example.

The NuSOnG beam design will be based on the one used by the NuTeV experiment, which is the most recent high energy, high statistics neutrino experiment. The experiment would use 800 GeV protons on target followed by a quad-focused, sign-selected magnetic beam-line. The beam flux, shown in Fig. 1, has very high neutrino or antineutrino purity ( $\sim 98 \%$ ) and small $\nu_{e}$ contamination ( $\sim 2 \%$ ) from kaon and muon decay. Using an upgraded Tevatron beam extraction it is expected that NuSOnG could collect $5 \times 10^{19}$ protons/yr, an increase by a factor of 20 from NuTeV . With this high intensity, such a new facility would also produce a neutrino beam from the proton dump having a sizable fraction of tau neutrinos for study.


Fig. 1. (Color online) The assumed energy-weighted flux ( $E d \phi / d E / 10^{6}$ POT) based on the NuTeV experiment in (a) neutrino mode (left) and (b) antineutrino mode (right). (a) In neutrino mode the fluxes are ordered: upper (black), muon neutrino; middle (blue), electron neutrino and antineutrino; lower (red), muon antineutrino. (b) In antineutrino mode the fluxes are ordered: upper (red), muon antineutrino; middle (blue), electron neutrino and antineutrino; lower (black), muon neutrino.

The baseline detector design is composed of a fine-grained target calorimeter for electromagnetic and hadronic shower reconstruction followed by a toroid muon spectrometer to measure outgoing muon momenta. The target calorimeter will be composed of $2,5002.5 \mathrm{~cm} \times 5 \mathrm{~m} \times 5 \mathrm{~m}$ glass planes interspersed with proportional tubes or scintillator planes. This gives a target which is made of isoscalar material with fine $1 / 4$ radiation length sampling. The detector will be composed of four target sections each followed by muon spectrometer sections and low mass decay regions to search for long-lived heavy neutral particles produced in the beam. The total length of the detector is $\sim 200 \mathrm{~m}$ and the fiducial mass for the four target calorimeter modules will be 3 kiloton which is 6 times larger than NuTeV or CHARM II. Figure 2 shows a simulated $\nu_{\mu}$ charged current event in the detector.

### 3.2. Description of $N u S O n G$ calibration beam

The requirements for NuSOnG calibration beam would be similar to those of NuTeV. Tagged beams of hadrons, electrons, and muons over a wide energy range $(5-200 \mathrm{GeV})$ would be required. The calibration beam will have the ability to be steered over the transverse face of the detector in order to map the magnetic field of each toroid with muons. Steering for hadrons and electrons would be less crucial than it was in NuTeV's case, but would still be useful.

The calibration beam can be constructed with a similar design to NuTeV . Upstream elements were used to select hadrons, electrons, or muons. An enhanced beam of electrons was produced by introducing a thin lead radiator into the beam and detuning the portion of the beam downstream of the radiator. A radiator was also used in the nominal beam tune to remove electrons. Particle ID (a threshold Cerenkov and TRD's) was incorporated in the spectrometer and used to tag


Fig. 2. A simulated muon neutrino, charged current event in the NuSOnG detector.
electrons when running at low energy. A pure muon beam was produced by introducing a 7 m long beryllium filter in the beam as an absorber.

The NuTeV calibration spectrometer determined incoming particle momenta with a precision of better than $0.3 \%$ absolute. ${ }^{14}$ The NuSOnG goal for calibrationbeam precision would be to measure energy scales to a precision of about $0.5 \%$, and we demonstrate (in later text of this paper) that this can be improved with fits to neutrino data.

For comparison, using the calibration beam, NuTeV achieved $0.43 \%$ precision on absolute hadronic energy scale and $0.7 \%$ on absolute muon energy scale (dominated by the ability to accurately determine the toroid map). Precise knowledge of the muon energy scale is especially important in order to achieve high measurement accuracy on the neutrino fluxes using the low- $\nu$ method. For example, a $0.5 \%$ precision on muon energy scale translates into about a $1 \%$ precision on the flux. Both energy scales are important for precision structure function measurements, and were the largest contributions to structure function measurement uncertainties in NuTeV. ${ }^{15}$

### 3.3. Experimental extraction of structure functions in $N u S O n G$

The high statistics of the NuSOnG experiment makes it possible to extract the structure functions directly from the $y$-distributions within bins of $\left(x, Q^{2}\right)$. Previous lower-statistics high-energy neutrino experiments either extracted structure functions by comparing the number of $\nu$ versus $\bar{\nu}$ events in an $\left(x, Q^{2}\right)$ bin, ${ }^{4}$ or by extracting the cross-sections $d \sigma / d y$ within the $\left(x, Q^{2}\right)$ bin and fitting for the structure functions using Eq. (1). ${ }^{15}$ Either method assumes a value for $R_{L}=\sigma_{L} / \sigma_{T}$ as
measured by other experiments, ${ }^{16}$ and depends on a measurement of the strange sea from dimuon events. ${ }^{17,18}$ With sufficient statistics, we can explore the possibility of measuring $x F_{3}^{\nu}\left(x, Q^{2}\right), x F_{3}^{\bar{\nu}}\left(x, Q^{2}\right), F_{2}\left(x, Q^{2}\right)$ and $R\left(x, Q^{2}\right)$ from the same data. ${ }^{10}$

Let us consider the cross-section of Eq. (1) as a function of $\left\{x F_{3}, F_{2}, R\right\}$; we denote this as $d \sigma^{\nu(\bar{\nu})}\left(x F_{3}, F_{2}, R\right)$, where the $\left(x, y, Q^{2}\right)$-dependence is assumed, and the structure functions can be different for neutrinos and antineutrinos. One can then fit for the structure functions $\left\{x F_{3}^{\mathrm{fit}}, F_{2}^{\mathrm{fit}}, R^{\text {fit }}\right\}$ in each $\left(x, Q^{2}\right)$ bin by minimizing the function

$$
\begin{equation*}
\chi^{2}=\sum_{\nu, \bar{\nu}} \sum_{y \text {-bins }} \frac{\left[N_{\mathrm{data}}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)-N_{\mathrm{MC}, \text { pred }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)\right]^{2}}{N_{\mathrm{data}}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)} . \tag{8}
\end{equation*}
$$

We will define the quantities of Eq. (8) in the following. Here, $N_{\text {data }}^{\nu(\bar{\nu})}$ is the number of $\nu$ or $\bar{\nu}$ data events in the $\left(x, y, Q^{2}\right)$ bin. To compute $\chi^{2}$, we first generate (gen) a sample of Monte Carlo events using an assumed set of structure functions $\left\{x F_{3}^{\text {gen }}, F_{2}^{\text {gen }}, R^{\text {gen }}\right\}$ to produce the cross-section $d \sigma^{\nu, \bar{\nu}}\left(x F_{3}^{\text {gen }}, F_{2}^{\text {gen }}, R^{\text {gen }}\right)$; we can then compute the number of generated events in each $\left(x, y, Q^{2}\right)$ bin, $N_{\mathrm{MC}, \mathrm{gen}}^{\nu(\bar{\nu})}$.

We next compute the predicted (pred) number of events in each $\left(x, y, Q^{2}\right)$ bin, $N_{\mathrm{MC}, \text { pred }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)$, by reweighting the Monte Carlo generated events as follows:

$$
\begin{equation*}
N_{\mathrm{MC}, \text { pred }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)=\sum_{\substack{\nu(\bar{\nu}) \text { events in } \\\left(x, y, Q^{2}\right) \text { bin }}} \frac{d \sigma^{\nu(\bar{\nu})}\left(x F_{3}^{\mathrm{fit}}, F_{2}^{\mathrm{fit}}, R^{\mathrm{fit}}\right)}{d \sigma^{\nu(\bar{\nu})}\left(x F_{3}^{\text {gen }}, F_{2}^{\text {gen }}, R^{\text {gen }}\right)} N_{\mathrm{MC}, \text { gen }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right) \tag{9}
\end{equation*}
$$

Here, $d \sigma^{\nu(\bar{\nu})}\left(x F_{3}^{\mathrm{fit}}, F_{2}^{\mathrm{fit}}, R^{\mathrm{fit}}\right)$ is the cross-section computed with the structure functions $\left\{x F_{3}^{\mathrm{fit}}, F_{2}^{\mathrm{fit}}, R^{\mathrm{fit}}\right\}$ which are the result of the $\chi^{2}$-minimization of Eq. (8). In principle, $\left\{x F_{3}^{\text {fit }}, F_{2}^{\text {fit }}, R^{\text {fit }}\right\}$ can be fit separately for the $\nu$ and $\bar{\nu}$ structure functions.

In the following, we will concentrate on the measurement of up to four separate structure functions, $\Delta x F_{3}\left(x, Q^{2}\right)=x F_{3}^{\nu}\left(x, Q^{2}\right)-x F_{3}^{\bar{\nu}}\left(x, Q^{2}\right), x F_{3}^{\text {avg }}=$ $\left(x F_{3}^{\nu}+x F_{3}^{\bar{\nu}}\right) / 2, F_{2}\left(x, Q^{2}\right)$ and $R\left(x, Q^{2}\right)$ where we assume that $F_{2}\left(x, Q^{2}\right)$ and $R\left(x, Q^{2}\right)$ are the same for neutrinos and antineutrinos; i.e. $F_{2}\left(x, Q^{2}\right)=F_{2}^{\nu}\left(x, Q^{2}\right)=$ $F_{2}^{\bar{\nu}}\left(x, Q^{2}\right)$ and $R\left(x, Q^{2}\right)=R^{\nu}\left(x, Q^{2}\right)=R^{\bar{\nu}}\left(x, Q^{2}\right)$.

### 3.4. Fitting for $\Delta x F_{3}$

We have studied the extraction of the structure function from the 600 million neutrino and 33 million antineutrino DIS events expected in the full NuSOnG data set. The dominant systematic error comes from the measurement of the muon momentum in the toroidal spectrometer. At NuTeV , the systematic uncertainty was $0.7 \%$ and we assume NuSOnG will achieve $0.5 \%$. Our studies are carried out by fitting the $y$-distribution in each $\left(x, Q^{2}\right)$ bin for $F_{2}$, the average value of $x F_{3}=x F_{3}^{\text {avg }}=\left(x F_{3}^{\nu}+x F_{3}^{\bar{\nu}}\right) / 2, \Delta x F_{3}=x F_{3}^{\nu}-x F_{3}^{\bar{\nu}}$ and $R$. In the first set of
studies, $R\left(x, Q^{2}\right)$ is set equal to the measured value ${ }^{16}$ and fits are done for the three structure functions, $F_{2}, x F_{3}^{\text {avg }}$ and $\Delta x F_{3}$.

Our fitting procedure begins with a set of Monte Carlo generated events, $N^{\text {gen }}\left(x, y, Q^{2}\right)$, sampled from the CCFR structure functions, and the nominal value for $\Delta x F_{3}$ from NuTeV, $\left\{F_{2}^{\text {nom }}, x F_{3}^{\text {nom }}\right\}$. We fit in bins of $\left(x, Q^{2}\right)$ as a function of $y$ and obtain the fit spectra by reweighting the original sample:

$$
\begin{aligned}
N^{\mathrm{fit}}\left(x, y, Q^{2}\right)= & \frac{F_{2}^{\mathrm{fit}}\left(x, Q^{2}\right)\left(2-2 y+y^{2} /(1+R)\right) \pm x F_{3}^{\mathrm{fit}}\left(x, Q^{2}\right)\left(1-(1-y)^{2}\right)}{F_{2}^{\mathrm{nom}}\left(x, Q^{2}\right)\left(2-2 y+y^{2} /(1+R)\right) \pm x F_{3}^{\text {nom }}\left(x, Q^{2}\right)\left(1-(1-y)^{2}\right)} \\
& \times N^{\mathrm{gen}}\left(x, y, Q^{2}\right),
\end{aligned}
$$

where the upper sign is for neutrinos and the lower for antineutrinos. In order to study the effects of the systematic energy scale shift, we produce a Monte Carlo sample where the muon energy scale is shifted by $0.5 \%, E_{\mu}^{\text {meas }}=1.005 E_{\mu}^{\text {true }}$, for each event. The fractional change in the number of events in each bin due to the energy scale shift is shown in Fig. 3.


Fig. 3. Fractional change in number of events for two characteristic $\left(x, Q^{2}\right)$ bins as a function of $y$. The fractional change comes from scaling the energy of each event by a factor of 1.005 .

This shifted event distribution, $N^{\text {shift }}\left(x, y, Q^{2}\right)$, is then used to carry out a three parameter fit to Eq. (8) where $F_{2}, x F_{3}^{\text {avg }}$, and $\Delta x F_{3}$ are varied. Large shifts in $\Delta x F_{3}$ result. For example, the shift from the input value in the $\left(x, Q^{2}\right)=$ $\left(0.08,12.6 \mathrm{GeV}^{2}\right)$ bin is $19.01 \%$, and the shift in other bins is even larger.

The effects of the energy scale uncertainty can be practically eliminated by including energy scale shift parameters in the fit. A muon energy scale change shifts the events in the various $y$-bins by an amount that is not consistent with that expected from changes in the structure functions. Therefore, fits to the $y$ distributions can isolate the effects of an energy scale shift and significantly reduce the structure function uncertainty from this systematic error. To estimate the systematic error reduction for this technique, three additional energy scale parameters are introduced in the fit to the $y$-distributions. These three parameters are used to produce an energy scale shift parametrization in each $\left(x, y, Q^{2}\right)$ bin given by

$$
E_{\mu \text { scale }}=E_{\mu \text { scale } 1}+E_{\mu \text { scale } 2} E_{\mu}+E_{\mu \text { scale } 3} E_{\mu}^{2}
$$

The updated prediction for the number of events in a given $\left(x, y, Q^{2}\right)$ bin is

$$
\begin{aligned}
N_{\mathrm{pred}}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)= & N_{\mathrm{MC}, \text { pred }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right) \\
& +E_{\mu \text { scale }}\left[N^{\mathrm{shift}}\left(x, y, Q^{2}\right)-N^{\mathrm{gen}}\left(x, y, Q^{2}\right)\right]
\end{aligned}
$$

and the $\chi^{2}$ used in the minimization is similar to Eq. (8) with the addition of pull terms associated with the three energy scale parameters

$$
\begin{align*}
\chi^{2}= & \sum_{\nu, \bar{\nu}} \sum_{y \text {-bins }} \frac{\left[N_{\text {data }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)-N_{\text {pred }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)\right]^{2}}{N_{\text {data }}^{\nu(\bar{\nu})}\left(x, y, Q^{2}\right)} \\
& +E_{\mu \text { scale } 1}+\frac{E_{\mu \text { scale } 2}}{(0.02)^{2}}+\frac{E_{\mu \text { scale } 3}}{(0.0002)^{2}} . \tag{10}
\end{align*}
$$

These pull terms correspond to an energy scale uncertainty of about $0.5 \%$ for muon energy values averaging between 50 and 70 GeV . This fitting technique renders the systematic error from the scale shift to be small in comparison with the statistical error. For example, in the bin $\left(x, Q^{2}\right)=\left(0.275,32 \mathrm{GeV}^{2}\right)$, the systematic error for $\Delta x F_{3}$ is $0.3 \%$ while the statistical error is $10 \%$; the value of the $E_{\mu \text { scale } 1}$ parameter is also determined to about $10 \%$.

In the ultimate analysis, the fit will be carried out simultaneously over all $x$ and $Q^{2}$ bins with one set of energy scale parameters. We have studied this using eight $x$ bins and six to eight $Q^{2}$ bins. Figure 4 shows the fractional error on $\Delta x F_{3}$ for different $x$ bins as a function of $Q^{2}$. In general, we believe NuSOnG can measure $\Delta x F_{3}$ over most of the ( $x, Q^{2}$ ) range to better than $10 \%$; in many cases around $3 \%$. Typical values for NuTeV are shown in two $x$ bins in Fig. 4. Since more than one $\left(x, Q^{2}\right)$ bin is being used to determine the energy scale shift parameters, the value of the $E_{\mu \text { scale 1 }}$ parameter can also be determined to about $3 \%$ from these fits.


Fig. 4. Fractional uncertainty for the fit value of $\Delta x F_{3}$ in different $x$ bins as a function of $Q^{2}$. The fit is to multiple $x$ and $Q^{2}$ bins extracting the three structure functions, $F_{2}, x F_{3}^{\text {avg }}$ and $\Delta x F_{3}$. For each of the fits, a global set of energy scale parameters is also determined from the fit. The dashed lines show the fractional error for the $\mathrm{NuTeV} 2 \mu$ measurement.

Simulation studies have also been made to estimate the uncertainties associated with doing fits to extract the four structure functions, $F_{2}, x F_{3}^{\text {avg }}, \Delta x F_{3}$ and $R$. The procedure is the same as used for the three structure function fits where the $\chi^{2}$ in Eq. (10) is minimized simultaneously over a number of $x$ and $Q^{2}$ bins with one set of energy scale parameters. In this case, the $\Delta x F_{3}$ and $R_{\text {long }}$ structure functions can be determined to between $5 \%$ and $20 \%$ for most of the $x$ and $Q^{2}$ range as shown in Figs. 5 and 6. The simulated $R_{\text {long }}$ measurements are shown in Fig. 7 along with previous measurements. ${ }^{16}$ As indicated from this figure, the capabilities of the NuSOnG to measure $R_{\text {long }}$ is much more precise that any previous experiment.

In summary, due to the very high statistics of a NuSOnG type experiment, an almost complete set of structure functions over a broad range of $x$ and $Q^{2}$ can be extracted from the data without introducing theoretical or experimental approximations. Further, systematic uncertainties that have limited the precision of previous structure function measurements can be eliminated by including fits to these uncertainties in the extraction procedure. We believe that with these techniques the structure function measurements will be statistics limited even for NuSOnG.

## 4. Nuclear Effects

Historically, neutrino experiments have played a major role in expanding our understanding of parton distribution functions through high statistics experiments such as CCFR, ${ }^{8}$ NuTeV, ${ }^{15,19,8}$ and CHORUS. ${ }^{20}$ However, the high statistics extract a price since the large event samples require the use of nuclear targets - iron in the case of both CCFR and NuTeV , and lead in the case of the CHORUS experiment. The problem is that if one wants to extract information on nucleon PDF's, then the effects of the nuclear targets must first be removed. NuSOnG can provide key measurements which will improve these corrections.

Charged lepton DIS has been measured on a wide range of targets. The most simplistic expectation for the structure functions might be that they would be given by an average of the appropriate number of proton and neutron results as in

$$
F_{2}^{A}\left(x, Q^{2}\right)=\frac{Z}{A} F_{2}^{P}\left(x, Q^{2}\right)+\frac{A-Z}{A} F_{2}^{n}\left(x, Q^{2}\right) .
$$

However, the results from a wide range of experiments show a much more complex behavior for the structure functions on nuclei. The typical behavior of the ratio of $F_{2}^{A}\left(x, Q^{2}\right)$ to $F_{2}^{d}\left(x, Q^{2}\right)$ where $d$ denotes a deuterium target shows four distinct regions as sketched in Fig. 8.

At small $x$ the ratio dips below one in what is called the shadowing region. At somewhat larger values of $x$ the ratio rises above one in the antishadowing region. At still larger values of $x$ the ratio again falls below one in the EMC region. Finally, as $x$ approaches one, Fermi motion smearing causes a significant rise in the ratio.


Fig. 5. Fractional uncertainty for the fit value of $\Delta x F_{3}$ in different $x$ bins as a function of $Q^{2}$. The fit is to multiple $x$ and $Q^{2}$ bins extracting the four structure functions, $F_{2}, x F_{3}^{\text {avg }}, \Delta x F_{3}$ and $R$. For each of the fits, a global set of energy scale parameters is also determined.


Fig. 6. Fractional uncertainty for the fit value of $R$ in different $x$ bins as a function of $Q^{2}$. The fit is to multiple $x$ and $Q^{2}$ bins extracting the four structure functions, $F_{2}, x F_{3}^{\text {avg }}, \Delta x F_{3}$ and $R$. For each of the fits, a global set of energy scale parameters is also determined.


Fig. 7. Extracted values of $R$ (labeled NuSOnG) from the four structure function fits as compared to previous measurements ${ }^{16}$ (labeled SLAC).


Fig. 8. Typical behavior of the ratio of the structure function on a nuclear target $A$ to that on a deuterium target.

This behavior shows only a modest dependence on $A$ for values above beryllium, with the shape remaining qualitatively the same and the amount of the suppression at $x \approx 0.6$ increasing slowly with $\log (A)$. Furthermore, there is little, if any, observed dependence on $Q^{2}$. These features are summarized nicely in the results shown in Ref. 21.

The mechanisms of nuclear scattering have also been studied theoretically. These mechanisms appear to be different for small and large Bjorken $x$ as viewed from the laboratory system. Bjorken $x$ is defined as $x=Q^{2} / 2 M \nu$, where $\nu$ and $\boldsymbol{q}$ are energy and momentum transfer to the target and $Q^{2}=\boldsymbol{q}^{2}-\nu^{2}$. The physical quantity which is responsible for the separation between large and small $x$ regions is a characteristic scattering time, which is also known as Ioffe time (or length) $\tau_{I}=\nu / Q^{2} .{ }^{22}$ If $\tau_{I}$ is smaller than the average distance between bound nucleons in a nucleus then the process can be viewed as incoherent scattering off bound nucleons. This happens at larger $x(>0.2)$.

### 4.1. Nuclear effects at small $\boldsymbol{x}$

We expect to find a difference between charged-lepton nucleus and neutrino nucleus scattering at small- $x$ because the space-time pictures for the two processes are different in this region. The underlying physical mechanism in the laboratory reference frame can be sketched as a two-stage process. At the first stage, the virtual photon $\gamma^{*}$, or $W^{*}$ or $Z^{*}$ in case of neutrino interactions, fluctuates into a quark-antiquark (or hadronic) state. In the second stage, this hadronic state then interacts with the
target. The uncertainty principle allows an estimate of the average lifetime of such hadronic fluctuation as

$$
\begin{equation*}
\tau=\frac{2 \nu}{m^{2}+Q^{2}}=\frac{1}{x M} \frac{Q^{2}}{m^{2}+Q^{2}}, \tag{11}
\end{equation*}
$$

where $m$ is the invariant mass of the hadrons into which the virtual boson converts, and $M$ is the proton mass. The same scale $\tau$ also determines characteristic longitudinal distances involved in the process. At small $x, \tau$ exceeds the average distance between bound nucleons. For this reason coherent multiple interactions of this hadronic fluctuation in a nucleus are important in the small- $x$ kinematic region. It is well known that the nuclear shadowing effect for structure functions is a result of coherent nuclear interactions of hadronic fluctuations of virtual intermediate boson. ${ }^{\text {b }}$

For neutrino interactions which are mediated by the axial-vector current, the fluctuation time $\tau$ is also given by Eq. (11). However, there are some open questions here; it was argued in Ref. 24 that the fluctuation and coherence lengths are not the same for the axial-vector current case. The experimental study of shadowing with neutrinos can provide an excellent test of the properties of the axial vector current, and the high energy of the NuSOnG beam will allow the kinematic reach and the resolution to study this phenomena. ${ }^{25}$

### 4.2. Nuclear effects in neutrino interactions

As there has been no systematic experimental study of $\nu$ and $\bar{\nu}$ nucleus interactions, one must then rely on theoretical models of the nuclear corrections. This is an unsatisfactory situation since one is essentially measuring quantities sensitive to the convolution of the the desired PDF's and unknown - or model dependent nuclear corrections.

As noted above, theoretically there are substantial differences between charged lepton and neutrino interactions on the same nucleus. There are other expected differences for neutrinos. For example, the relative nuclear shadowing effects for the structure function $F_{3}$ is predicted to be substantially different from that for $F_{2} .{ }^{26}$ This is because the structure function $F_{3}$ describes the correlation between the vector and the axial-vector current in neutrino scattering. In terms of helicity cross-sections, the structure function $F_{3}$ is given by the cross-section asymmetry between the left- and right-polarized states of a virtual $W$ boson. It is known that such a difference of cross-sections is strongly affected by Glauber multiple scattering corrections in nuclei. ${ }^{27-29}$ This causes an enhanced nuclear shadowing effect for the structure function $F_{3}$.

It is important to experimentally address the question of nuclear effects in neutrino scattering so that the neutrino data can be used in proton fits without bringing

[^293]

Fig. 9. Comparison between the reference fit and the unshifted CHORUS and NuTeV neutrino data without any nuclear corrections.
in substantial nuclear uncertainties. For example, in a recent analysis ${ }^{30}$ the impact of new neutrino data on global fits for PDF's was assessed. The conclusion reached in this analysis was that the uncertainties associated with nuclear corrections precluded using the neutrino data to constrain the nucleon PDF's. If NuSOnG can address these uncertainties, then the neutrino data can play an even more prominent role in the global fits to the proton PDF.

Furthermore, nuclear effects are interesting in their own right. Parametrizations of nuclear PDF's on various targets exist in the literature. However, there is no universally accepted model which describes these nuclear corrections over the entire range of $x$ from first principles. This makes it difficult to generalize the above behavior observed in charged lepton DIS to DIS with $\nu$ or $\bar{\nu}$ beams. Models such as that in Ref. 31 exist, but to date there have been no high statistics studies of $\nu$ or $\bar{\nu}$ DIS over a wide range of nuclear targets with which to test them.

A study presented in Ref. 30 examined the role of new lepton pair production data from E-866 and new neutrino DIS data from the NuTeV and CHORUS collaborations in global fits for nucleon PDF's. For the actual fitting of the PDF's it was necessary to include nuclear corrections for the neutrino and antineutrino cross-sections and the model of Ref. 31 was used. As a byproduct of that analysis, it was possible to compare a reference fit, obtained without using data on nuclear targets, to the neutrino and antineutrino data in order to obtain an estimate of what the nuclear corrections should look like. This comparison is shown in Fig. 9.

This figure shows some results from Ref. 30 in the form of "data/theory" averaged over $Q^{2}$ and presented versus $x$. The results are from a global fit but are plotted without the model-dependent nuclear corrections which were used in
the fit (the neutrino data were not used in the reference fit). It is notable that the overall pattern of deviations shown in Fig. 9 are, in general, similar to that seen in charged lepton DIS as sketched in Fig. 8. However, the deviations from unity are perhaps smaller. At high $x$, the effect of Fermi smearing is clear. At moderate $x$ the EMC effect is observable. It is interesting to note that there is no clear indication of a turnover at low $x$ in the shadowing region for $\nu$ data. Also, note the striking similarity between the $\nu$ and $\bar{\nu}$ results. This appears to imply that the differences in the nuclear effects between neutrino and antineutrino DIS are small. As discussed later, when we consider $\Delta x F_{3}$ and isospin violation, it is crucial to model differences in the nuclear effects between $\nu$ and $\bar{\nu}$ scattering as a function of $x$.

To make progress in understanding nuclear corrections in neutrino interactions, access to high statistics data on a variety of nuclear targets will be essential. This will allow the $A$-dependence to be studied as a function of both $x$ and $Q^{2}$, as has been done in charged lepton deep inelastic scattering. PDF's from global fits without the neutrino data can then be used to make predictions to be compared with the $A$-dependent $\nu$ and $\bar{\nu}$ cross-sections, thereby allowing the nuclear corrections to be mapped out for comparison with theoretical models.

The primary target of NuSOnG will be $\mathrm{SiO}_{2}$. However, we can investigate a range of $A$-values by replacing a few slabs of glass with alternative target materials: $\mathrm{C}, \mathrm{Al}, \mathrm{Fe}$ and Pb . This range of nuclear targets would both extend the results of MINER $\nu$ A to the NuSOnG kinematic region, and provide a check (via the Fe target) against the NuTeV measurement.

Given the NuSOnG neutrino flux, we anticipate $58 k \nu$-induced and $30 k \bar{\nu}$ induced CC DIS events per ton of material. A single ton would be sufficient to extract $F_{2}(x)$ and $x F_{3}(x)$ averaged over all $Q^{2}$; a single $5 \mathrm{~m} \times 5 \mathrm{~m} \times 2.54 \mathrm{~cm}$ slab of any of the above materials will weigh more than that. The use of additional slabs would permit further extraction of the structure functions into separate ( $x, Q^{2}$ ) bins as was done in the NuTeV analysis, at the potential expense of complicating the shower energy resolution in the subdetectors containing the alternative targets; this issue will be studied via simulation.

Table 2 shows that two 50 -module stacks would be sufficient to accumulate enough statistics on alternative nuclear targets for a full structure-function extraction for each material. However, for basic cross-section ratios in $x$, a single slab of each would suffice.

Table 2. Alternative target materials for cross-section analysis.

| Material | Mass of <br> 2.54 cm slab (tons) | Number of slabs needed <br> for <br> NuTeV-equivalent statistics |
| :---: | :---: | :---: |
| C | 1.6 | 33 |
| Al | 1.9 | 27 |
| Fe | 5.5 | 10 |
| Pb | 7.9 | 7 |

### 4.3. Measuring nuclear effects with the MINER $A$ and NuSOnG detectors

The MINER $\nu \mathrm{A}$ experiment will also be studying neutrino induced nuclear effects and will be starting its initial physics run in early 2010. To study nuclear effects in MINER $\nu$ A, a cryogenic vessel containing liquid helium ( 0.2 ton fiducial mass) will be installed upstream of the MINER $\nu$ A detector. ${ }^{\text {c }}$ Within the MINER $\nu$ A detector, solid carbon, iron and lead targets will be installed upstream of the pure scintillator active detector. The total mass is 0.7 ton of $\mathrm{Fe}, 0.85$ ton of $\mathrm{Pb}, 0.4$ ton of He and somewhat over 0.15 ton of C. Since the pure scintillator active detector essentially acts as an additional $3-5$ ton carbon target $(\mathrm{CH})$, the pure graphite $(\mathrm{C})$ target is mainly to check for consistency. For a run consisting of $4.0 \times 10^{20} \mathrm{POT}$ in the NuMI Low Energy (LE) beam and $12 \times 10^{20}$ POT in the NuMI Medium Energy (ME) beam, MINER $\nu$ A would collect over 2 M events on $\mathrm{Fe}, 2.5 \mathrm{M}$ events on $\mathrm{Pb}, 600 \mathrm{~K}$ on helium and 430 K events on C as well as 9.0 M events on the scintillator within the fiducial volume.

Studying nuclear effects with the NuSOnG detector will involve fewer nuclear targets but considerably more statistics on each. In addition, the much higher energy of the incoming neutrinos with NuSOnG means a much wider kinematic range of study. In particular, NuSOnG will have a much higher $Q^{2}$ for a given low- $x$ to study shadowing by neutrinos and will be able to measure the shadowing region down to much smaller $x$ for the same $Q^{2}$ range as MINER $\nu$ A. A significant addition to the study of nuclear effects with neutrinos would be the addition of a large, perhaps active ("Bubble Chamber"), cryogenic target containing hydrogen or deuterium. With the intense NuSOnG neutrino beam, a significant sample of neutrino-hydrogen and neutrino-deuterium events could provide the normalization we need to further unfold nuclear effects in neutrino-nucleus interactions.

## 5. QCD Fits

The extraction of up to six structure functions from the cross-sections of neutrino and antineutrino DIS discussed so far (cf. Eq. (1)) has been completely modelindependent relying only on some fundamental principles such as Lorentz-invariance of the cross-section and gauge-invariance of the hadronic tensor which is expanded in terms of the structure functions which parametrize the unknown hadronic physics.

More can be said about the structure functions in QCD. While it is still not possible to accurately compute the $x$-dependence of the structure functions from first principles, QCD allows us to derive renormalization group equations (RGE's) which relate the structure functions at different (perturbative) scales $Q$. Note that the structure functions at the scale $Q$ can be directly related to structure functions at a different scale $Q_{0}$ (see, e.g. Eqs. (5.58) and (5.76) in Ref. 33). However, it

[^294]is more convenient to work in the QCD-improved parton model where the RGE's governing the scale-dependence of the parton distribution functions (PDF's) are the familiar DGLAP evolution equations; these can also be used to compute the structure functions at $Q$ given the PDF's at that scale. ${ }^{34-36}$ Furthermore, this approach has the crucial advantage that the universal PDF's allow us to make predictions for other observables as well. In addition to the $Q$-dependence, the QCD calculations provide certain (approximate) relations between different structure functions as will be visible from the parton model expressions below.

In this section we will discuss the analysis of the cross-section data within the framework of the QCD-improved parton model. Already in the past, high statistics measurements of neutrino DIS on heavy nuclear targets (CCFR, NuTeV, Nomad, CHORUS ...) have attracted much interest in the literature since they provide valuable information for global fits of PDF's. ${ }^{37,38}$

Due to the weak nature of neutrino interactions, the use of nuclear targets is unavoidable; this complicates the extraction of free nucleon PDF's, because modeldependent corrections must be applied to the data (cf. Sec. 4). Of course, these same data are also useful for extracting the nuclear parton distribution functions (NPDF's) and for such an analysis no nuclear correction factors are required. Conversely, the NPDF's can be utilized to compute the required nuclear correction factors within the QCD parton model. ${ }^{39}$ Similar to proton PDF's, universal nuclear PDF's are needed for the description of many processes with nuclei in the initial state. This involves physics at other neutrino experiments, heavy ion colliders (RHIC, LHC), and a possible future electron-ion collider (EIC).

The NuSOnG experiment will have two orders of magnitude higher statistics than the NuTeV and CCFR experiments (over an extended kinematic range), and so it will be possible to study small effects such as the strangeness asymmetry with better precision, or to establish for the first time isospin violation in the light quark sector. Better understanding these effects is relevant for improving the extraction of the weak mixing angle in a Paschos-Wolfenstein-type analysis.

### 5.1. PDF's

NuSOnG will perform measurements on different nuclear targets. The PDF's for a nucleus $(A, Z)$ are constructed as

$$
\begin{equation*}
f_{i}^{A}(x, Q)=\frac{Z}{A} f_{i}^{p / A}(x, Q)+\frac{(A-Z)}{A} f_{i}^{n / A}(x, Q) \tag{12}
\end{equation*}
$$

In the following discussion we take into account deviations from isospin symmetry, a nonvanishing strangeness asymmetry, and the possibility to have nonisoscalar targets. For this purpose we introduce the following linear combinations of strange quark PDF's:

$$
\begin{equation*}
s^{+, A}=s^{A}+\bar{s}^{A}, \quad s^{-, A}=s^{A}-\bar{s}^{A}, \tag{13}
\end{equation*}
$$

where the strangeness asymmetry is described by a nonvanishing PDF $s^{-}$. Note however that we continue to assume $s^{p / A}=s^{n / A}$ and $\bar{s}^{p / A}=\bar{s}^{n / A}$. Also, we neglect any possible charm asymmetry, i.e. we use $c^{A}=\bar{c}^{A}$ such that $c^{-, A}=c^{A}-\bar{c}^{A}=0$ and $c^{+, A}=c^{A}+\bar{c}^{A}=2 c^{A}$.

Deviations from isospin symmetry can be parametrized in the following way:

$$
\begin{array}{ll}
\delta u_{v}^{p / A}=u_{v}^{p / A}-d_{v}^{n / A}, & \delta d_{v}^{p / A}=d_{v}^{p / A}-u_{v}^{n / A}, \\
\delta \bar{u}^{p / A}=\bar{u}^{p / A}-\bar{d}^{n / A}, & \delta \bar{d}^{p / A}=\bar{d}^{p / A}-\bar{u}^{n / A} . \tag{15}
\end{array}
$$

These definitions allow us to write the PDF's in a way which makes deviations from isoscalarity and isospin symmetry manifest:

$$
\begin{align*}
& 2 u_{v}^{A}=\left[u_{v}^{p / A}+d_{v}^{p / A}-\delta d_{v}^{p / A}\right]-\Delta\left[u_{v}^{p / A}-d_{v}^{p / A}+\delta d_{v}^{p / A}\right],  \tag{16}\\
& 2 d_{v}^{A}=\left[u_{v}^{p / A}+d_{v}^{p / A}-\delta u_{v}^{p / A}\right]+\Delta\left[u_{v}^{p / A}-d_{v}^{p / A}-\delta u_{v}^{p / A}\right],  \tag{17}\\
& 2 \bar{u}^{A}=\left[\bar{u}^{p / A}+\bar{d}^{p / A}-\delta \bar{d}^{p / A}\right]-\Delta\left[\bar{u}^{p / A}-\bar{d}^{p / A}+\delta \bar{d}^{p / A}\right],  \tag{18}\\
& 2 \bar{d}^{A}=\left[\bar{u}^{p / A}+\bar{d}^{p / A}-\delta \bar{u}^{p / A}\right]+\Delta\left[\bar{u}^{p / A}-\bar{d}^{p / A}-\delta \bar{u}^{p / A}\right], \tag{19}
\end{align*}
$$

where $\Delta=(N-Z) / A$ parametrizes the deviation from isoscalarity. We have written Eqs. (16)-(19) so that the r.h.s. is expressed explicitly in terms of proton PDF's and the four $\delta$-terms $\left\{\delta u_{v}^{p / A}, \delta d_{v}^{p / A}, \delta \bar{u}^{p / A}, \delta \bar{d}^{p / A}\right\}$; the $\delta$-terms vanish individually if isospin symmetry is preserved.

### 5.2. Structure functions

The structure functions for a nuclear target $(A, Z)$ are given by

$$
\begin{equation*}
F_{i}^{A}(x, Q)=\frac{Z}{A} F_{i}^{p / A}(x, Q)+\frac{(A-Z)}{A} F_{i}^{n / A}(x, Q) \tag{20}
\end{equation*}
$$

such that they can be computed in next-to-leading order as convolutions of the nuclear PDF's with the conventional Wilson coefficients, i.e. generically

$$
\begin{equation*}
F_{i}^{A}(x, Q)=\sum_{k} C_{i k} \otimes f_{k}^{A} . \tag{21}
\end{equation*}
$$

In order to discuss which information can be extracted from a high statistics measurement of neutrino and antineutrino DIS cross-sections, we briefly review the parton model expressions for the 6 structure functions. For simplicity, we first restrict ourselves to leading order, neglect heavy quark mass effects (as well as the associated production thresholds), and assume a diagonal CKM matrix. In our numerical results, these effects are taken into account.

The neutrino-nucleus structure functions are given by (suppressing the dependence on $x$ and $Q^{2}$ ):

$$
\begin{align*}
& F_{1}^{\nu A}=d^{A}+s^{A}+\bar{u}^{A}+\bar{c}^{A}+\cdots  \tag{22}\\
& F_{2}^{\nu A}=2 x F_{1}^{\nu A}  \tag{23}\\
& F_{3}^{\nu A}=2\left[d^{A}+s^{A}-\bar{u}^{A}-\bar{c}^{A}+\cdots\right] . \tag{24}
\end{align*}
$$

The structure functions for antineutrino scattering are obtained by exchanging the quark and antiquark PDF's in the corresponding neutrino structure functions:

$$
\begin{equation*}
F_{1,2}^{\bar{\nu} A}=F_{1,2}^{\nu A}[q \leftrightarrow \bar{q}], \quad F_{3}^{\bar{\nu} A}=-F_{3}^{\nu A}[q \leftrightarrow \bar{q}] . \tag{25}
\end{equation*}
$$

Explicitly this gives

$$
\begin{align*}
& F_{1}^{\bar{\nu} A}=u^{A}+c^{A}+\bar{d}^{A}+\bar{s}^{A}+\cdots,  \tag{26}\\
& F_{2}^{\bar{\nu} A}=2 x F_{1}^{\bar{\nu} A},  \tag{27}\\
& F_{3}^{\bar{\nu} A}=2\left[u^{A}+c^{A}-\bar{d}^{A}-\bar{s}^{A}+\cdots\right] . \tag{28}
\end{align*}
$$

The longitudinal structure function can be obtained with the help of the following relation:

$$
\begin{equation*}
F_{L}^{\nu A}=r^{2} F_{2}^{\nu A}-2 x F_{1}^{\nu A}=\frac{4 x^{2} M^{2}}{Q^{2}} F_{2}^{\nu A} \tag{29}
\end{equation*}
$$

where $r^{2}=1+4 x^{2} M^{2} / Q^{2}$. Finally, it is customary to introduce the ratio of longitudinal to transverse structure functions:

$$
\begin{equation*}
R_{L}^{\nu A}=\frac{F_{L}^{\nu A}}{2 x F_{1}^{\nu A}}=\frac{r^{2} F_{2}^{\nu A}}{2 x F_{1}^{\nu A}}-1=\frac{4 x^{2} M^{2}}{Q^{2}} . \tag{30}
\end{equation*}
$$

Similar equations hold for antineutrino scattering. At leading order (LO) it is clear that $R_{L}^{\nu}=R_{L}^{\bar{\nu}}$. Figure 10 displays $R_{L}^{\nu,(\bar{\nu})}$ for both LO and NLO; we observe that at NLO the difference between $R_{L}^{\nu}$ and $R_{L}^{\bar{\nu}}$ can be neglected in the following discussion.


Fig. 10. Structure function ratio $R_{L}$ for neutrino and antineutrino nucleon $\left.(N=(p+n) / 2)\right)$ scattering at $Q^{2}=20 \mathrm{GeV}^{2}$. The solid and dashed lines show NLO results obtained with the GRV98 PDF's, ${ }^{40}$ while the dotted line shows the LO result of Eq. (30).

### 5.3. Constraints on the PDF's

The differential cross-section in Eq. (1) can be written as

$$
\begin{equation*}
\frac{d \sigma}{d x d y}=K\left[A+B(1-y)^{2}+C y^{2}\right] \tag{31}
\end{equation*}
$$

with $K=\frac{G_{F}^{2} M E}{2 \pi\left(1+Q^{2} / M_{W}^{2}\right)^{2}}, A=F_{2} \pm x F_{3}, B=F_{2} \mp x F_{3}$ and $C=\frac{2 x^{2} M^{2}}{Q^{2}} F_{2}-F_{L}$ where the upper sign refers to neutrino and the lower one to antineutrino scattering. This form of $d \sigma$ shows that the (anti)neutrino cross-section data naturally encodes information on the four structure function combinations $F_{2}^{\nu A} \pm x F_{3}^{\nu A}$ and $F_{2}^{\bar{\nu} A} \pm$ $x F_{3}^{\bar{\nu}} A$ in separate regions of the phase space. In addition, at large $y$ the structure function combination $C$ contributes. However, to good accuracy $C^{\nu}=C^{\bar{\nu}}$ so that $C$ drops out in the difference of neutrino and antineutrino cross-sections.

Assuming $s^{A}=\bar{s}^{A}$ and $c^{A}=\bar{c}^{A}$, the structure functions $F_{2}^{\nu A}$ and $F_{2}^{\bar{\nu} A}$ constrain the valence distributions $d_{v}^{A}=d^{A}-\bar{d}^{A}, u_{v}^{A}=u^{A}-\bar{u}^{A}$ and the flavor-symmetric sea $\Sigma^{A}:=\bar{u}^{A}+\bar{d}^{A}+\bar{s}^{A}+\bar{c}^{A}+\cdots$ via the relations:

$$
\begin{align*}
& \frac{1}{x} F_{2}^{\nu A}=2\left[d_{v}^{A}+\Sigma^{A}\right]  \tag{32}\\
& \frac{1}{x} F_{2}^{\bar{\nu} A}=2\left[u_{v}^{A}+\Sigma^{A}\right] \tag{33}
\end{align*}
$$

Furthermore, we have

$$
\begin{align*}
& \frac{1}{x} F_{2}^{\nu A}+F_{3}^{\nu A}=4\left(d^{A}+s^{A}\right),  \tag{34}\\
& \frac{1}{x} F_{2}^{\bar{\nu} A}-F_{3}^{\bar{\nu} A}=4\left(\bar{d}^{A}+\bar{s}^{A}\right) . \tag{35}
\end{align*}
$$

Since we constrain the strange distribution utilizing the dimuon data, the latter two structure functions are useful to separately extract the $d^{A}$ and $\bar{d}^{A}$ distributions.

For an isoscalar nucleus we encounter further simplifications. In this case, $u^{A}=$ $d^{A}$ and $\bar{u}^{A}=\bar{d}^{A}=: \bar{q}^{A}$ which implies $u_{v}^{A}=d_{v}^{A}=: v^{A}$. Hence, the independent quark distributions are $\left\{v^{A}, \bar{q}^{A}, s^{A}=\bar{s}^{A}, c^{A}=\bar{c}^{A}, \ldots\right\}$. In particular, we have $F_{2}^{\nu A}=F_{2}^{\bar{\nu} A}$ for an isoscalar target such that our original set of 6 independent structure functions reduces to three independent functions (say $F_{2}^{\nu A}, F_{3}^{\nu A}, F_{3}^{\bar{\nu} A}$ ) under the approximations made.

In a more refined analysis, allowing for a nonvanishing strangeness asymmetry and isospin violation we can evaluate the nonsinglet structure function $\Delta F_{2}^{\nu} \equiv$ $F_{2}^{\nu A}-F_{2}^{\bar{\nu} A}$ with the help of the relations in Eqs. (16)-(19):

$$
\begin{equation*}
\Delta F_{2}^{\nu}=2 x s^{-, A}+x \delta d_{v}^{p / A}-x \delta u_{v}^{p / A}+\Delta x\left[2 u_{v}^{p / A}-2 d_{v}^{p / A}+\delta d_{v}^{p / A}-\delta u_{v}^{p / A}\right] . \tag{36}
\end{equation*}
$$

For a nuclear isoscalar target $(Z=N=A / 2, \Delta=0)$ this expression simplifies to

$$
\begin{equation*}
\Delta F_{2}^{\nu}=2 x s^{-, A}+x \delta d_{v}^{p / A}-x \delta u_{v}^{p / A} \tag{37}
\end{equation*}
$$

As one can see, $\Delta F_{2}^{\nu}$ will be small and sensitive to the strangeness asymmetry and isospin violating terms for the valence quarks.

The difference of the neutrino and antineutrino cross-sections provides, in principle, access to this quantity:

$$
\begin{equation*}
\frac{d^{2} \sigma^{\nu} A}{d x d y}-\frac{d^{2} \sigma^{\bar{\nu}} A}{d x d y} \simeq K\left[\Delta F_{2}^{\nu}+x F_{3}^{\nu}+(1-y)^{2}\left(\Delta F_{2}^{\nu}-x F_{3}^{\nu}\right)\right] \tag{38}
\end{equation*}
$$

with $F_{3}^{\nu}=F_{3}^{\nu A}+F_{3}^{\bar{\nu} A}$.
It is important to note that in the global fit to extract structure functions we do not make use of the above simplifications, but instead we perform a complete $\chi^{2}$-analysis of all neutrino and antineutrino cross-section data.

## 6. Isospin (Charge Symmetry) Violation and $\Delta x F_{3}$

The question of isospin violation is central to the PW electroweak measurement. In the NuTeV analysis, isospin symmetry was assumed. As discussed in Ref. 3, various models which admit isospin violation can pull the $\mathrm{NuTeV} \sin \theta_{W}$ measurement toward the Standard Model. However it would take significantly larger isospin violation to bring NuTeV into agreement with the rest of the world's data. Better constraints of isospin violation will be crucial to the interpretation of the NuSOnG results.

When we relate DIS measurements from heavy targets such as ${ }_{26}^{56} \mathrm{Fe}$ (used in NuTeV ) or ${ }_{82}^{207} \mathrm{~Pb}$ (CHORUS) back to a proton or isoscalar target, we generally make use of isospin symmetry where we assume that the proton and neutron PDF's can be related via a $u \leftrightarrow d$ interchange. While isospin symmetry is elegant and well motivated, the validity of this exact charge symmetry must ultimately be established by experimental measurement. There have been a number of studies investigating isospin symmetry violation; ${ }^{41-47}$ therefore, it is important to be aware of the magnitude of potential violations of isospin symmetry and the consequences on the extracted PDF components. For example, the naive parton model relations are modified if we have a violation of exact $p \leftrightarrow n$ isospin-symmetry, or charge symmetry violation (CSV); e.g. $u^{n}(x) \not \equiv d^{p}(x)$ and $u^{p}(x) \not \equiv d^{n}(x)$.

It is noteworthy that a violation of isospin symmetry is automatically generated once QED effects are taken into account. ${ }^{48-50}$ This is because the photon couples to the up quark distribution $u^{p}(x)$ differently than to the down quark distribution $d^{n}(x)$. These terms can be as much as a few percent in the medium $x$ range, see e.g. Fig. 1 in Ref. 50.

Combinations of structure functions can be particularly sensitive to isospin violations, and NuSOnG is well suited to measure some of these observables. For example, residual $u, d$-contributions to $\Delta x F_{3}=x F_{3}^{\nu}-x F_{3}^{\bar{\nu}}$ from charge symmetry violation would be amplified due to enhanced valence components $\left\{u_{v}(x), d_{v}(x)\right\}$, and because the $d \rightarrow u$ transitions are not subject to slow-rescaling corrections which suppress the $s \rightarrow c$ contribution to $\Delta x F_{3} \cdot{ }^{43}$ Here the ability of NuSOnG to separately measure $x F_{3}^{\nu}$ and $x F_{3}^{\bar{\nu}}$ over a broad kinematic range will provide powerful constraints on the sensitive structure function combination $\Delta x F_{3}$.

Separately, the measurement of $\Delta F_{2} \equiv \frac{5}{18} F_{2}^{\mathrm{CC}}\left(x, Q^{2}\right)-F_{2}^{\mathrm{NC}}\left(x, Q^{2}\right)$ in Charged Current (CC) $W^{ \pm}$exchange and Neutral Current (NC) $\gamma / Z$ exchange processes can also constrain CSV; ${ }^{45}$ because NuSOnG will measure $F_{2}^{\mathrm{CC}}$ on a variety of targets, this will reduce the systematics associated with the heavy nuclear target corrections thus providing an additional avenue to study CSV.

In the following, we provide a detailed analysis of CSV which also investigates the various experimental systematics associated with each measurement. We shall find it is important to consider all the systematics which impact the various experimental measurements to assess the discriminating power.

## 6.1. $\Delta x F_{3}$ and isospin violations

We recall the leading-order relations of the neutrino structure function $F_{3}$ on a general nuclear target:

$$
\begin{align*}
& \frac{1}{2} F_{3}^{\nu A}(x)=d^{A}+s^{A}-\bar{u}^{A}-\bar{c}^{A}+\cdots  \tag{39}\\
& \frac{1}{2} F_{3}^{\bar{\nu} A}(x)=u^{A}+c^{A}-\bar{d}^{A}-\bar{s}^{A}+\cdots \tag{40}
\end{align*}
$$

where $A$ represents the nuclear target $A=\{p, n, d, \ldots\}$, and the "..." represent higher-order contributions and terms from the third generation $\{b, t\}$ quarks. Note that to illustrate the general features of these processes, we use a schematic notation as in Eqs. (39) and (40); for the numerical calculations, the full NLO expressions are employed including mass thresholds, "slow-rescaling" variables, target mass corrections, and CKM elements where appropriate.

For a nuclear target $A$ we can construct $\Delta x F_{3}^{A}$ as

$$
\begin{align*}
\Delta x F_{3}^{A}= & x F_{3}^{\nu A}-x F_{3}^{\bar{\nu} A} \\
= & 2 x \Delta\left[\left(u^{p / A}-d^{p / A}\right)+\left(\bar{u}^{p / A}-\bar{d}^{p / A}\right)+\frac{1}{2} \delta I^{A}\right] \\
& +2 x s^{+, A}-2 x c^{+, A}+x \delta I^{A}+\mathcal{O}\left(\alpha_{S}\right) \tag{41}
\end{align*}
$$

where $\mathcal{O}\left(\alpha_{S}\right)$ represents the higher-order QCD corrections, and the isospin violations are given by $\delta I^{A}$ :

$$
\begin{equation*}
\delta I^{A}=\delta d-\delta u+\delta \bar{d}-\delta \bar{u} \tag{42}
\end{equation*}
$$

For a flux-weighted linear combination of $F_{3}^{\nu}$ and $F_{3}^{\bar{\nu}}$, terms proportional to the strange quark asymmetry can enter Eq. (41), cf. Refs. 45, 46 and 41. For a signselected $\nu / \bar{\nu}$ beam as for NuTeV or NuSOnG, this complication is not necessary. As before, we have defined $s^{ \pm, A}(x)=\left[s^{A}(x) \pm \bar{s}^{A}(x)\right]$ and $c^{ \pm, A}(x)=\left[c^{A}(x) \pm \bar{c}^{A}(x)\right]$.

In the limit of isospin symmetry, all four terms on the r.h.s. of Eq. (42) vanish individually. For a nuclear isoscalar target, $Z=N=A / 2$, we can construct $\Delta x F_{3}$ from the above:

$$
\begin{equation*}
\Delta x F_{3}=x F_{3}^{\nu A}-x F_{3}^{\bar{\nu} A}=2 x s^{+, A}-2 x c^{+, A}+x \delta I^{A}+\mathcal{O}\left(\alpha_{S}\right) . \tag{43}
\end{equation*}
$$

Note in Eq. (41) that for a nuclear target $A$ which is close to isoscalar, we have $Z \sim N$ such that the up and down quark terms are suppressed; this is a benefit of the NuSOnG glass $\left(\mathrm{SiO}_{2}\right)$ target which is very nearly isoscalar. More specifically, for $\mathrm{SiO}_{2}$ we have $Z(\mathrm{O})=8, Z(\mathrm{Si})=14, m(\mathrm{O})=15.994, m(\mathrm{Si})=28.0855$. Using $A=Z+N$ we have $(N-Z) / A=(A-2 Z) / A$ for the prefactor in Eq. (41) which yields $(N-Z) / A \sim-0.000375$ for O and $(N-Z) / A \sim 0.00304$ for Si.

In Eq. (41) the PDF's $\left\{u^{p / A}, d^{p / A}, \ldots\right\}$ represent quark distributions bound in a nucleus $A$. With a single nuclear target, we can determine the CSV term $\delta I^{A}$ for this specific $A$; measurements on different nuclear targets would be required in order to obtain the $A$ dependence of $\delta I^{A}$ if we need to scale to a proton or isoscalar target.

Thus, an extraction of any isospin violation $\delta I^{A}$ requires a careful separation of these contributions from the strange, charm, and higher-order terms. Theoretical NLO calculations for $\Delta x F_{3}$ are available; thus the $\mathcal{O}\left(\alpha_{S}\right)$ corrections can be addressed. Additionally, NuSOnG can use the dimuon process $\left(\nu N \rightarrow \mu^{+} \mu^{-} X\right)$ to constrain the strange sea.

In conclusion we find that while this is a challenging measurement, NuSOnG's high statistics measurement of $\Delta x F_{3}$ should provide a window on CSV which is relatively free of large experimental systematics. We emphasize that $\Delta x F_{3}$ may be extracted from a single target, thereby avoiding the complications of introducing nuclear corrections associated with different targets. This is in contrast to the other measurements discussed below. However, if we desire to rescale the $\delta I^{A}$ effects to a different nucleus $A$, then multiple targets would be required.

### 6.2. Measurement of $\Delta F_{2} \equiv \frac{5}{18} F_{2}^{\mathrm{CC}}\left(x, Q^{2}\right)-F_{2}^{\mathrm{NC}}\left(x, Q^{2}\right)$

A separate determination of CSV can be achieved using the measurement of $F_{2}$ in CC and NC processes via the relation:

$$
\begin{align*}
\Delta F_{2} \equiv & \frac{5}{18} F_{2}^{\mathrm{CC}, A}\left(x, Q^{2}\right)-F_{2}^{\mathrm{NC}, A}\left(x, Q^{2}\right) \\
\simeq & \frac{1}{6} x \frac{(N-Z)}{A}\left[\left(u^{p / A}-d^{p / A}\right)+\left(\bar{u}^{p / A}-\bar{d}^{p / A}\right)\right] \\
& +\frac{1}{6} x s^{+, A}(x)-\frac{1}{6} x c^{+, A}(x)+\frac{1}{6} x \frac{N}{A} \delta I^{A}+\mathcal{O}\left(\alpha_{s}\right) \tag{44}
\end{align*}
$$

with the definitions

$$
F_{2}^{\mathrm{CC}, A}=\frac{1}{2}\left[F_{2}^{\nu A}+F_{2}^{\bar{\nu} A}\right], \quad F_{2}^{\mathrm{NC}, A}=F_{2}^{\ell A}
$$

In Eq. (44), the first term is proportional to $(N-Z) / A$ which vanishes for an isoscalar target. The second and third terms are proportional to the heavy quark distributions $s^{+, A}$ and $c^{+, A}$. The next term is the CSV contribution which is proportional to $\delta I^{A}$ given in Eq. (42). It is curious that this has the same form as the CSV contribution for $\Delta x F_{3}$ of Eq. (41). Finally, the last term represents the higher-order QCD corrections.

While the character of the terms on the l.h.s. of Eqs. (43), (44) are quite similar, the systematics of measuring $\Delta F_{2}$ may differ substantially from that of $\Delta x F_{3}$. For example, the measurement of $\Delta F_{2}$ requires the subtraction of structure functions from two entirely different experiments. The CC neutrino-nucleon data are extracted from heavy nuclear targets (to accumulate sufficient statistics); as such, these data are generally subject to large nuclear corrections so that the heavy targets can be related to the isoscalar $N=\frac{1}{2}(p+n)$ limit. Conversely, the NC charged-lepton-nucleon process proceeds via the electromagnetic interaction. Therefore sufficient statistics can be obtained for light targets including $H$ and $D$ and no large heavy target corrections are necessary. Therefore, we must use the appropriate nuclear correction factors when we combine $F_{2}^{\mathrm{CC}}$ and $F_{2}^{\mathrm{NC}}$, and this will introduce a systematic uncertainty.

Separately, the heavy quark production mechanism is different in the CC and NC processes. Specifically, in the CC case we encounter the process $s+W^{+} \rightarrow c$ where the charm mass threshold kinematics must be implemented. On the other hand, the NC process is $c+\gamma \rightarrow c$ which is proportional to the charm sea distribution and has different threshold behavior than the CC process. Even though the charm production process is modeled at NLO, the theoretical uncertainties which this introduces can dominate precision measurements.

### 6.3. Other measurements of CSV

We very briefly survey other measurements of CSV in comparison to the above.
The measurement of the lepton charge asymmetry in $W$ decays from the Tevatron can constrain the up and down quark distributions. ${ }^{51,52}$ In this case, the extraction of CSV constraints is subtle; while isospin symmetry is not needed to relate $p$ and $\bar{p}$, this symmetry is typically used in a global fit of the PDF's to reduce data on heavy targets to $p$.

In the limit that all the data in the analysis were from proton targets, CSV would not enter; hence this limit only arises indirectly from the mix of targets which enter a global fit. At present, while much of the data does come from proton targets (H1, ZEUS, CDF, D0), there are some data sets from both $p$ and $d$ (BCDMS, NMC, E866), and some that use heavier targets (E-605, NuTeV). ${ }^{30,53}$ Thus, an outstanding question is if CSV were present, to what extent would this be "absorbed" into a global fit. The ideal procedure would be to parametrize the CSV and include this in a global analysis. While this step has yet to be implemented, there is a recent effort to include the nuclear corrections as a dynamic part of a global fit. ${ }^{39}$

Additionally, NMC measures $F_{2}^{n} / F_{2}^{p}$ data which has an uncertainty of order a few percent. ${ }^{54}$ There are also fixed-target Drell-Yan experiments such as NA51 ${ }^{47}$ and $\mathrm{E} 866^{55}$ which are sensitive to the ratio $\bar{d} / \bar{u}$ in the range $0.04<x<0.27$. We will soon have LHC data $(p p)$ to add to our collection, thus providing additional constraints in a new kinematic region.

### 6.4. Conclusions on charge symmetry violation

NuSOnG will be able to provide high statistics DIS measurements across a wide $x$ range. Because the target material $\left(\mathrm{SiO}_{2}\right)$ is nearly isoscalar, this will essentially allow a direct extraction of the isoscalar observables.
$\Delta x F_{3}$ is one of the cleaner measurements of CSV in terms of associated experimental systematic uncertainties as this measurement can be extracted from a single target. The challenge here will be to maximize the event samples, and the NuSOnG high statistics will play an important role in this regard.

The measurement of $\Delta F_{2}$ is more complicated as this must combine measurements from both CC and NC experiments which introduces nuclear correction factors. ${ }^{56,39}$ Since NuSOnG will provide high statistics $F_{2}^{\mathrm{CC}}$ measurements for a variety of $A$ targets, this will yield an alternate handle on the CSV and also improve our understanding of the associated nuclear corrections.

The combination of these high statistics measurements, together with external constraints, will yield important information on this fundamental symmetry.

## 7. Measurements of the Heavy Quarks

### 7.1. Measurement of the strange sea

Charged current neutrino-induced charm production, $(\nu / \bar{\nu}) N \rightarrow \mu^{+} \mu^{-} X$, proceeds primarily through the subprocesses $W^{+} s \rightarrow c$ and $W^{-} \bar{s} \rightarrow \bar{c}$ (respectively), so this provides a unique mechanism to directly probe the $s(x)$ and $\bar{s}(x)$ distributions. Approximately $10 \%$ of the charmed particles decay into $\mu+X$, adding a second oppositely signed muon in the CC event final state. These "dimuon" events are easily distinguishable, and make up approximately $1 \%$ of the total CC event sample. Hence, the recent high statistics dimuon measurements ${ }^{17,57,18,58,59}$ play an essential role in constraining the strange and antistrange components of the proton. On NuSOnG, the dimuon data will be used in the same manner.

Distinguishing the difference between the $s(x)$ and $\bar{s}(x)$ distributions,

$$
\begin{equation*}
s^{-}(x) \equiv s(x)-\bar{s}(x), \tag{45}
\end{equation*}
$$

is necessary for the PW style analysis. This analysis is sensitive to the integrated strange sea asymmetry,

$$
\begin{equation*}
S^{-} \equiv \int_{0}^{1} x s^{-}(x) d x \tag{46}
\end{equation*}
$$

through its effect on the denominator of the PW ratio, as has been recognized in numerous references. ${ }^{60-64}$

Note that the quantity $\int_{0}^{1} s^{-}(x) d x$ must vanish as the proton carries no net strangeness. Indeed, this condition is a strong constraint on the form of the strange quark distributions. It requires that $s^{-}(x)$ have at least one sign change, which can be see in Fig. 11 at small $x$.


Fig. 11. NuTeV measurement of $x s^{-}(x)$ vs $x$ at $Q^{2}=16 \mathrm{GeV}^{2}$. Outer band is combined errors, inner band is without $B_{c}$ uncertainty.

The highest precision study of $s^{-}$to date is from the NuTeV experiment. ${ }^{57,65}$ The sign selected beam allowed measurement of the strange and antistrange seas independently, recording 5163 neutrino-induced dimuons, and 1380 antineutrino induced dimuon events in its iron target. Figure 11 shows the fit for the asymmetry between the strange and antistrange seas in the NuTeV data.

The integrated strange sea asymmetry from NuTeV has a positive central value: $0.00196 \pm 0.00046$ (stat) $\pm 0.00045$ (syst) $)_{-0.00107}^{+0.00148}$ (external). In NuSOnG, as in NuTeV , the statistical error will be dominated by the antineutrino data set and is expected to be about 0.0002 . The systematic error is dominated by the $\pi$ and $K$ decay-in-flight subtraction. This can be addressed in NuSOnG through test-beam measurements which will allow a more accurate modeling of this background, as well as applying the techniques of CCFR to constrain this rate. ${ }^{66-68}$ We expect to be able to reduce this error to about 0.0002 . The combination of these reduces the total error by about $10 \%$, because the main contribution comes from the external inputs.

The external error on the measurement is dominated by the error on the average charm semimuonic branching ratio, $B_{c}$ :

$$
\begin{equation*}
B_{c}=\Sigma_{i} \int \phi(E) f_{i}(E) B_{\mu-i} d E \tag{47}
\end{equation*}
$$

where $\phi$ is the neutrino flux in energy bins, $f_{i}$ is the energy dependent production fraction for each hadron, and $B_{\mu-i}$ is the semimuonic branching ratio for each hadron. In the NuTeV analysis, this is an external input, with an error of about $10 \%$. To make further progress, this error must be reduced.


Fig. 12. World measurements of $B_{c}$. See Refs. 17, 69-71, 59, 58, 72.

Figure 12 shows the world measurements of $B_{c}$, taken from Refs. 17, 69-71, $59,58,72$. Measuring $B_{c}$ directly requires the capability to resolve the individual charmed particles created in the interaction. The best direct measurements are from experiments using emulsion detectors (E531, CHORUS) where the decay of the charmed meson is well tagged. ${ }^{71,72}$ Since the cross-section for charmed meson production is energy dependent, it is important to make a measurement near the energy range of interest. The NuTeV strange sea asymmetry study used a re-analysis of 125 charm events measured by the FNAL E531 experiment ${ }^{71}$ in the energy range of the NuTeV analysis $\left(E_{\nu}>20 \mathrm{GeV}\right) . B_{c}$ has also been constrained through indirect measurement via fits.

For NuSOnG, our goal is to reduce the error on $B_{c}$ using an in situ measurement on glass by at least a factor of 1.5 . One method is to include $B_{c}$ as a fit parameter in the analysis of the dimuon data. The unprecedented high statistics will allow a fit as a function of neutrino energy for the first time. Dimuons from high $x$ neutrino DIS almost exclusively result from scattering off valence quarks, such that the dimuon cross-section in that region isolates $B_{c}$ from the strange sea. In dimuon fits, the assumption is that $B_{c-\nu}=B_{c-\bar{\nu}}, B_{c}$ may be measured directly from the dimuon data.

Unfortunately, the antineutrino charm production process is not well measured by past experiments; hence, there is concern that the assumption $B_{c-\nu}=B_{c-\bar{\nu}}$ may not be accurate. For example, the fact that the process $\nu n \rightarrow \mu^{-} \Lambda_{c}$ has no analogous reaction in the antineutrino channel may lead to a difference in the neutrino and antineutrino branching ratios.

These arguments provide the motivation for including a high resolution target/ tracker in the NuSOnG design that can directly measure the semileptonic branching ratio to charm in both $\nu$ and $\bar{\nu}$ running modes. There are two feasible detector technologies. The first is to use emulsion, as in past experiments; this is proven technology and scanning could be done at the facility in Nagoya, Japan. The second is to use the NOMAD-STAR detector ${ }^{73,74}$ or a similar design. This is a 45 kg silicon vertex detector which ran in front of the NOMAD experiment. The target was boron carbide interleaved with the silicon. This detector successfully measured 45 charm events in that beam, identifying $D^{+}, D^{0}$ and $D_{s}$. A similar detector of this size in the NuSOnG beam would yield about $900 \nu$ events and $300 \bar{\nu}$ events. This has the advantage of being a low- $Z$ material which is isoscalar and close in mass to the $\mathrm{SiO}_{2}$ of the detector.

### 7.2. Strange quark contribution to the proton spin

An investigation of the strange quark contribution to the elastic vector and axial form factors of the proton is possible in NuSOnG, by observing NC elastic and CC quasielastic scattering events; namely $\nu p \rightarrow \nu p$ and $\nu n \rightarrow \mu^{-} p$ events in neutrino mode, and $\bar{\nu} p \rightarrow \bar{\nu} p$ and $\bar{\nu} p \rightarrow \mu^{+} n$ events in antineutrino mode. The motivation for making this measurement comes from a number of recent (and not so recent) studies of proton structure.

Over the last 15 years a tremendous effort has been made at MIT-Bates, Jefferson Lab, and Mainz to measure the strange quark contribution to the vector form factors (that is, the electromagnetic form factors) of the proton via parity-violating electron scattering from protons, deuterons, and ${ }^{4} \mathrm{He} .{ }^{75-85}$ The technique is to observe the parity-violating beam spin asymmetry in elastic scattering of longitudinally polarized electrons from these unpolarized targets; this asymmetry is caused by an interference between the one-photon and one- $Z$ exchange amplitudes. ${ }^{86}$ As a result, the weak neutral current analog of the electromagnetic form factors of the proton may be measured and this gives access to the strange quark contribution. This worldwide experimental program will soon be complete. The results available to date (from global analyses ${ }^{87-89}$ ) indicate a small (and nearly zero) contribution of the strange quarks to the elastic electric form factor, $G_{E}^{s}$; this is not surprising, as the total electric charge in the proton due to strange quarks is zero. At the same time, these same data point to a small but likely positive contribution of the strange quarks to the elastic magnetic form factor, $G_{M}^{s}$, indicating a small positive contribution of the strange quarks to the proton magnetic moment. Due to the prominent role played by the $Z$-exchange amplitude, these experiments are also sensitive to the strange quark contribution to the elastic axial form factor, which is related to the proton spin structure.

It is now well established by leptonic deep inelastic scattering experiments that the spins of the valence and sea quarks in the proton together contribute about $30 \%$ of the total proton intrinsic angular momentum of $\hbar / 2$. The strange quark
contribution is estimated to be about $-10 \%$ for inclusive DIS (an analysis which makes use of $\mathrm{SU}(3)$-flavor symmetry), ${ }^{90}$ but is found to be approximately zero in semiinclusive DIS (an alternative analysis which makes no use of $\mathrm{SU}(3)$ but needs fragmentation functions instead). ${ }^{91} \mathrm{~A}$ recent global analysis ${ }^{92}$ made use of both inclusive and semiinclusive DIS, and allowed for the possibility of SU(3)-flavor violation; this analysis found no need for any violation of $\operatorname{SU}(3)$, and also concluded that the strange quark contribution to the proton spin was small and negative. In the deep inelastic context, the contribution of the strange quarks to the proton spin is encapsulated in the spin-dependent strange quark parton distribution function,

$$
\Delta s(x)=s^{\rightarrow}(x)-s^{\leftarrow}(x)
$$

where $s^{\rightarrow}(x)\left[s^{\leftarrow}(x)\right]$ is the probability density for finding a strange quark of momentum fraction $x$ with its spin parallel [antiparallel] to the proton spin. The axial current relates the first moment of this parton distribution function to the elastic axial form factor of the proton, ${ }^{93} G_{A}^{s}$, at $Q^{2}=0$ :

$$
\int_{0}^{1} d x \Delta s(x)=G_{A}^{s}\left(Q^{2}=0\right) .
$$

The strange quark contribution to the elastic axial form factor can be measured by combining data from neutrino NC elastic scattering from the proton with data from parity-violating elastic $\overrightarrow{e p}$ scattering. ${ }^{94}$ In this way the strange quark contribution to the proton spin can be measured in a completely independent way using low$Q^{2}$ elastic scattering instead of high- $Q^{2}$ deep inelastic scattering. An analysis done using this method ${ }^{87}$ indicates that $G_{A}^{s}$ may in fact be negative at $Q^{2}=0$, but this conclusion is not definitive due to the limitations of the currently available neutrino data.

Since the neutrino experiments will undoubtedly be carried out on nuclear targets (perhaps carbon or argon), then the extraction of the strangeness form factors of the proton from these data needs to be done with care. Recent theoretical investigations suggest that ratio of NC to CC events is an ideal observable as the nuclear effects appear to largely cancel in this ratio. ${ }^{95}$ This is an area where the improved nuclear corrections discussed in Sec. 4 would prove a valuable cross check on these measurements.

The only available data on neutrino NC elastic scattering is from the BNL E734 experiment; ${ }^{96}$ the uncertainties reported from that experiment are considerable, and therefore limit the accuracy of any extraction of $G_{A}^{s}$ based on this data. If NuSOnG can provide more precise measurements of NC elastic scattering extended to lower $Q^{2}$ values, then the promise of this analysis technique can be fulfilled. Since the integrated luminosity of NuSOnG will be very much larger, far more statistics will be collected on the NC elastic process than in BNL E734. As this process has not been modeled for the proposed NuSOnG detector with a detailed Monte Carlo calculation, we cannot make any quantitative statement about the systematic uncertainties at present.

### 7.3. Measurements of the charm sea

### 7.3.1. Charm production

We can also study the charm-sea component of the proton which can arise from the gluon splitting process $g \rightarrow c \bar{c}$ producing charm constituents inside the proton. ${ }^{97-99}$ In a measurement complementary to the above strange sea extraction, the charm sea, $c(x, \mu)$, can be measured using the following process:

$$
\begin{aligned}
\nu_{\mu}+c \rightarrow \nu_{\mu}+ & c \\
& \hookrightarrow s+\mu^{+}+\nu_{\mu}
\end{aligned}
$$

In this process, we excite a constituent charm quark in the proton via the NC exchange of a $Z$ boson; the final state charm quark then decays semileptonically into $s \mu^{+} \nu_{\mu}$. We refer to this process as Wrong Sign Muon (WSM) production as the observed muon is typically the opposite sign from the expected $\nu_{\mu} d \rightarrow \mu^{-} u$ DIS process. For antineutrino beams, there is a complementary process $\bar{\nu}_{\mu}+\bar{c} \rightarrow \bar{\nu}_{\mu}+\bar{c}$ with a subsequent $\bar{c} \rightarrow \bar{s}+\mu^{-}+\bar{\nu}_{\mu}$ decay with yields a WSM with respect to the conventional $\bar{\nu}_{\mu} u \rightarrow \mu^{+} d$ process. Here, the ability of NuSOnG to have sign-selected beams is crucial to this measurement as it allows us to distinguish the secondary muons, and thus extract the charm-sea component.

In the conventional implementation of the heavy quark PDF's, the charm quark becomes an active parton in the proton when the scale $\mu$ is greater than the charm mass $m_{c}$; i.e. $f_{c}(x, \mu)$ is nonzero for $\mu>m_{c}$. Additionally, we must "rescale" the Bjorken $x$ variable as we have a massive charm in the final state. The original rescaling procedure is to make the substitution $x \rightarrow x\left(1+m_{c}^{2} / Q^{2}\right)$ which provides a kinematic penalty for producing the heavy charm quark in the final state. ${ }^{100}$ As the charm is pair-produced by the $g \rightarrow c \bar{c}$ process, there are actually two charm quarks in the final state - one which is observed in the semileptonic decay, and one which decays hadronically and is part of the hadronic shower. Thus, the appropriate rescaling is not $x \rightarrow x\left(1+m_{c}^{2} / Q^{2}\right)$ but instead $x \rightarrow \chi=x\left(1+4 m_{c}^{2} / Q^{2}\right)$; this rescaling is implemented in the ACOT- $\chi$ scheme, for example. ${ }^{101-103}$ The factor $\left(1+4 m_{c}^{2} / Q^{2}\right)$ represents a kinematic suppression factor which will suppress the charm process relative to the lighter quarks.

The differential cross-section for NC neutrino scattering is
$\frac{d \sigma}{d x d y}(\nu p \rightarrow \nu c)=\frac{G_{F}^{2} M_{N} E_{\nu}}{\pi} R_{Z}^{2}\left(Q^{2}\right)\left[g_{L}^{2}+g_{R}^{2}(1-y)^{2}-\frac{1}{2}\left(2 g_{L} g_{R}\right) \frac{M_{N}}{E_{\nu}}\right] \xi c(\xi, \mu)$,
where $g_{L}=t_{3}-Q_{c}^{2} \sin ^{2} \theta_{W}, g_{R}=-Q_{c}^{2} \sin ^{2} \theta_{W}$, and for charm $t_{3}=1 / 2$ and $Q_{c}=2 / 3$. The factor $R_{Z}\left(Q^{2}\right)=1 /\left(1+Q^{2} / M_{Z}^{2}\right)$ arises from the $Z$-boson propagator. The corresponding result for the anticharm is given with the substitutions $g_{L} \leftrightarrow g_{R}$ and $c \leftrightarrow \bar{c}$.

In the limit we can neglect the $M_{N} / E_{\nu}$ term, we have the approximate expressions for the total cross-section: ${ }^{98}$

$$
\begin{equation*}
\sigma(\nu p \rightarrow \nu c) \sim \frac{G_{F}^{2} M_{N} E_{\nu}}{\pi}(0.129) C \tag{48}
\end{equation*}
$$

and

$$
\begin{equation*}
\sigma(\nu p \rightarrow \nu \bar{c}) \sim \frac{G_{F}^{2} M_{N} E_{\nu}}{\pi}(0.063) \bar{C} \tag{49}
\end{equation*}
$$

with $C=\int_{\xi_{\text {min }}}^{1} \xi c(\xi, \mu) d \xi$ and $\bar{C}=\int_{\xi_{\text {min }}}^{1} \xi \bar{c}(\xi, \mu) d \xi$. We take $\xi=x\left(1+4 m_{c}^{2} / Q^{2}\right)$ and $\xi_{\text {min }}=m_{c}^{2} /\left(2 M_{N} \nu\right)$.

We will be searching for the WSM signal compared to the conventional CC DIS process; therefore it is useful to benchmark the rate for WSM production by comparing this to the usual CC DIS process,

$$
\begin{equation*}
\frac{d \sigma}{d x d y}\left(\nu p \rightarrow \mu^{-} X\right)=\frac{G_{F}^{2} M_{N} E_{\nu}}{\pi} R_{W}^{2}\left(Q^{2}\right)\left[q(x)+(1-y)^{2} \bar{q}(x)\right] \tag{50}
\end{equation*}
$$

with $R_{W}\left(Q^{2}\right)=1 /\left(1+Q^{2} / M_{W}^{2}\right)$. We can again integrate over $x$ and $y$ to obtain an estimate of the total cross-section in terms of the integrated PDF's as in Eqs. (48) and (49):
$\sigma\left(\nu N \rightarrow \mu^{-} X\right) \sim \frac{G_{F}^{2} M_{N} E_{\nu}}{\pi} R_{W}^{2}\left(Q^{2}\right) \frac{1}{2}\left[U+D+2 S+\frac{1}{3}(\bar{U}+\bar{D}+2 \bar{C})\right]$,
where $\{U, D, S\}$ are defined analogously to $C$, and we have used $N=\frac{1}{2}(p+n)$ for an isoscalar target.

The relative rate for NC charm production is determined by the above factors together with a ratio of integrated PDF's. For a mean neutrino energy of 100 GeV , the massive charm cross-section is down a factor of $\sim 0.005$ compared to the total inclusive cross-section. As the muon from the NC charm process is a secondary muon, we must additionally fold in the semileptonic branching ratio $B_{c} \sim 10 \%$, and the acceptance factor of observing the secondary muon in the detector $\left(A_{\mu} \sim 20 \%\right) .{ }^{17}$ Combining the relevant factors, we estimate the rate for NC charm production is approximately a factor of $10^{-4}$ as compared to the CC DIS process. Thus, for an anticipated design of $600 \mathrm{M} \nu_{\mu}$ CC events, one would expect on the order of 60 K NC charm events. This estimate is also consistent with a direct scaling from the NuTeV result of Ref. 99.

### 7.3.2. Backgrounds

Extrapolating from investigations by CCFR, ${ }^{98}$ and $\mathrm{NuTeV},{ }^{99}$ the dominant background for the measurement of the charm sea comes from $\bar{\nu}_{\mu}$ contamination. In these studies, it was determined that by demanding $E_{\text {vis }}>100 \mathrm{GeV}$, the background rate could be reduced to $2.3 \times 10^{-4}$. Other background processes include $\nu_{e}$ induced dilepton production, misidentified dimuon events, and NC interactions with a $\pi / K$ decay in the hadron shower; these processes contribute approximately an additional $1.5 \times 10^{-4}$ to the background rate. As compared to CCFR and NuTeV , the NuSOnG design has a number of improvements such as lower mass density for improved shower measurement; hence, comparable background reductions should be achievable.


Fig. 13. Integrated momentum fractions $\int_{0}^{1} x f_{i}(x, Q)$ of charm (upper curve) and bottom (lower curve) PDF's (in percent) vs $Q$ in GeV . Both the quark and antiquark contributions are included. Horizontal lines at $0.5 \%$ and $1.0 \%$ are indicated as this is the typical size of postulated intrinsic contributions.

### 7.3.3. Intrinsic charm

In the above discussion we have assumed that the charm component of the proton arises perturbatively from gluons splitting into charm quark pairs, $g \rightarrow c \bar{c}$; in this scenario the charm PDF typically vanishes at scales below the charm mass $\left(f_{c}\left(x, \mu<m_{c}\right)=0\right)$, and for $\mu>m_{c}$ all the charm partons arise from gluon splitting.

There is an alternative picture where the charm quarks are taken to be intrinsic to the proton; in this case there are intrinsic charm partons present at scales $\mu<m_{c}$. For $\mu>m_{c}$, the charm PDF is then a combination of this "intrinsic" PDF and the "extrinsic" PDF component arising from the $g \rightarrow c \bar{c}$ process.

A number of analyses have searched for an intrinsic charm component of the proton, and this intrinsic component is typically constrained to have an integrated momentum fraction less than a percent or two. ${ }^{104,105}$

In Fig. 13 we display the integrated momentum fraction, $\int_{0}^{1} x f_{i}(x, \mu)$, for charm and bottom as a function of $\mu$ due to the "extrinsic" PDF component arising from the $g \rightarrow c \bar{c}$ or $g \rightarrow b \bar{b}$ process. These momentum fractions start from zero at the corresponding quark mass, and increase slowly as the partonic components pick up momentum from the gluon splitting process.

If we are searching for an additional intrinsic component with a momentum fraction of $\sim 1 \%$, we will be most sensitive to such a component in the threshold region where the "intrinsic" component is not overwhelmed by the "extrinsic" contribution. In this regard, NuSOnG is well suited to search for these intrinsic terms as it will provide good statistics in the threshold region. Measuring the charm production process described above, NuSOnG can attempt to extract the charm PDF as a function of the $\mu$ scale, and then evolve back to $\mu=m_{c}$. Three outcomes are possible:
(i) $f_{c}\left(x, \mu=m_{c}\right)<0$, which would imply the data are inconsistent with the normal QCD evolution. ${ }^{\text {d }}$
(ii) $f_{c}\left(x, \mu=m_{c}\right)=0$, which would imply the data is consistent with no intrinsic charm PDF.
(iii) $f_{c}\left(x, \mu=m_{c}\right)>0$, which would imply the data is consistent with an intrinsic charm PDF.

By making accurate measurements of charm induced processes in the threshold region, NuSOnG can provide a discriminating test to determine which of the above possibilities is favored. Hence, the high statistics of NuSOnG in the threshold region are well suited to further constrain the question of an intrinsic charm component.

## 8. Summary and Conclusions

The NuSOnG experiment can search for "new physics" from the keV through TeV energy scales. This article has focused mainly on the QCD physics which can be accessed with this new high energy, high statistics neutrino scattering experiment. During its five-year data acquisition period, the NuSOnG experiment could record almost one hundred thousand neutrino-electron elastic scatters and hundreds of millions of DIS events, exceeding the current world data sample by more than an order of magnitude.

With this wealth of data, NuSOnG can address a wide variety of topics including the following.

- NuSOnG can increase the statistics of the Elastic Scattering (ES) and Deeply Inelastic Scattering (DIS) data sets by nearly two orders of magnitude.
- The unprecedented statistics of NuSOnG allow the possibility to perform separate extractions of the structure functions: $\left\{F_{2}^{\nu}, x F_{3}^{\nu}, R_{L}^{\nu}, F_{2}^{\bar{\nu}}, x F_{3}^{\bar{\nu}}, R_{L}^{\bar{\nu}}\right\}$. This allows us to test many of the symmetries and assumptions which were employed in previous structure function determinations.
- NuSOnG will help us to disentangle the nuclear effects which are present in the PDF's. Furthermore, this may help us address the long-standing tensions between the NC charged-lepton and CC neutrino DIS measurements.
- High precision NuSOnG measurements are sensitive to Charge Symmetry Violation (CSV) and other "new physics" processes. Such effects can significantly influence precision Standard Model parameter extractions such as $\sin \theta_{W}$. In particular, $\Delta x F_{3}$ is a sensitive probe of both the heavy quark components, and CSV effects.
- NuSOnG dimuon production provides an exceptional probe of the strange quark PDF's, and the sign-selected beam can separately study $s(x)$ and $\bar{s}(x)$. Additionally, NuSOnG can probe the $s$-quark contribution to the proton spin.

[^295]- The high statistics of NuSOnG may allow the measurement of the charm sea and an method to prove the intrinsic-charm content of the proton. While this is a difficult measurement, the NuSOnG kinematics allow the measurement of charm-induced processes in the threshold region where the "intrinsic" character can most easily be discerned.

While the above list presents a very compelling physics case for NuSOnG, this is only a subset of the full range of investigations that can be addressed with this facility.

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$$
\begin{array}{ll}
\left|\eta_{e}\right|<2.5 & p_{T, e}>20 \mathrm{GeV} \\
M_{\perp, W}>20 \mathrm{GeV} & p_{T, \nu}>20 \mathrm{GeV} \\
\left|\eta_{j}\right|<4.5 & p_{T, j}>25 \mathrm{GeV}
\end{array}
$$

Table 12: Summary of the cuts applied in the analysis.


Fig. 56: The average number of jets as a function of $p_{T, W}$ (left) and $p_{T, j_{1}}$ (right). The $p_{T, W}$ plot shows the $B H S$ exclusive sums prediction, while the $p_{T, j_{1}}$ plot is obtained from $S$-MEPS.

### 17.3 RESULTS OF THE COMPARISON

In this section, we compare the results of different theoretical descriptions for $W+n$-jets production at the LHC. The number $n$ can take values from 2 and above, as we will mostly consider inclusive samples. The four descriptions, which we will compare here in more detail, are

- the $B H S$ calculation of $W+2$-jets at NLO,
- the combined sample of $W+2,3,4$-jet events at NLO from $B H S$, as described in the 17.2 section,
- the $S$-MEPS merged $W+n$-jets sample using LO tree-level matrix elements up to $n=5$, and
- the approach of $H E J$.

Throughout this study, we will consider inclusive samples of $W^{-}$boson production in association with at least two hard jets identified by the anti- $k_{T}$ jet algorithm using $R=0.4$. The jets are required to have $p_{T, j}>25 \mathrm{GeV}$. We look only in the $W^{-} \rightarrow e^{-} \bar{\nu}_{e}$ decay channel and use the cuts given in Tab. 12 where $M_{\perp, W}$ is defined as $M_{\perp, W}=\sqrt{\left(\left|\vec{p}_{T, e}\right|+\left|\vec{p}_{T, \nu}\right|\right)^{2}-\left(\vec{p}_{T, e}+\vec{p}_{T, \nu}\right)^{2}}$.

The HEJ predictions use the geometric mean of the jet transverse momenta to determine the renormalisation and factorisation scale, i.e. $\left(\prod p_{T, j}\right)^{1 / n}$. This central choice will be varied by a factor of two in either direction to provide an envelope (marked by dotted lines in the corresponding figures) around the HEJ default prediction. The BHS predictions instead use $\hat{H}_{T}^{\prime} / 2$ as the NLO calculation becomes unstable for a scale which is too low. In the $S$-MEPS calculation, scales are chosen according to the default prescription given by ME\&TS [426].

The variables $H_{T, 2}, p_{T, W}$ and $p_{T, j_{1}}$ are less sensitive to the presence of additional radiation than $H_{T}$, as discussed in the introduction. The plots, which we present in Figs. 56 and 57 address the alternative question: given a particular value of $H_{T}, H_{T, 2}$ etc. how many jets are typically found in the event?

Figs. 56 and 57 show the stacked results for the average number of jets as a function of $p_{T, W}, p_{T, j_{1}}$, $H_{T}$ and $H_{T, 2}$ visualising the contributions from each exclusive 2,3,4-jet sample and the inclusive 5 -jet


Fig. 57: The contribution from different multiplicities to the average number of jets as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the BHS exclusive sums prediction, while the lower ones are extracted from S-MEPS.
sample. The left (right) plot in Fig. 56 and the upper (lower) rows of plots in Fig. 57 depict the results as obtained from the combined BHS sample (the $S$-MEPS sample). In all cases the different colours correspond to the terms in the numerator of the formula for the average number of jets,

$$
\begin{equation*}
\langle N\rangle_{5}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{106}
\end{equation*}
$$

where blue, green, red and magenta stand for $i=2,3,4$ and $i=5$, respectively. The subscript to $\langle N\rangle$ clarifies that we truncate the determination of the average after the fifth jet bin, noting that $\langle N\rangle_{k} \rightarrow\langle N\rangle$ for a sufficiently large number of jet bins. This makes no difference for the BHS predictions employed here since the jet multiplicity de facto is limited to five, but it does for the $S$-MEPS and HEJ computations where events with $i>5$ jets do occur. We have defined $n_{k}^{\text {exc } / \mathrm{inc}}=d \sigma_{k}^{\text {exc } / \mathrm{inc}} / d O$ where $O$ denotes an observable like $H_{T}$, or $\Delta y$ presented later on. Note that in Fig. 57 the 5 -jet part contributes to the average number of jets with a factor of 5 , while the 2 -jet part, for example, contributes with a factor of 2 only.

The layout of Fig. 58 (including the colour coding) is the same as before: here, we however display, wrt. $n_{2}^{\text {inc }}$, the relative fractions of the different multiplicities corresponding to the terms in the denominator of Eq. (106). In other words, in Fig. 58 we consider the partitioning of

$$
\begin{equation*}
1=\frac{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{107}
\end{equation*}
$$



Fig. 58: The fraction of the total rate from different multiplicities as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the $B H S$ exclusive sums prediction, while the lower ones are extracted from $S$-MEPS.

Although there is just a $30 \%$ fraction of inclusive 5 -jet events to the total cross section, we observe that their contribution to the build-up of $\langle N\rangle\left(H_{T}\right)$ for very large $H_{T}$ gets close to $50 \%$. Also, for an $H_{T} \sim$ 500 GeV , the average number of jets is composed evenly between the 2,3 -jet and 4,5 -jet contributions, while the relative fraction of the 2,3 -jet events is nearly $70 \%$. This emphasizes the dominance of multijet events in forming large $H_{T}$ values. It also can be seen that for medium $H_{T}$ values, $400<H_{T}<$ 700 GeV , all the multiplicities give roughly the same contribution to the variable $\langle N\rangle\left(H_{T}\right)$, while for low $H_{T}$, the average is primarily described by 2-jet events.

Going clockwise through Figs. 56 and 57 we see that the average number of jets is indeed sensitive to higher multiplicities when considered as a function of $p_{T, W}, p_{T, j_{1}}$ and $H_{T, 2}$, but in all these cases this happens to a lesser extent as if considered as a function of $H_{T}$. As expected, the dependence is mildest for $p_{T, W}$, the most inclusive observable studied here. We also observe that the jet-bin decomposition of $p_{T, j_{1}}$ and $H_{T, 2}$ turns out very similar. Most strikingly we note the increase in the contribution from the highest multiplicity events, the ones containing more or at least five jets. For $H_{T, 2}$, we furthermore display to the right of Fig. 58 the relative fractions as done in the $H_{T}$ case. Even for largest $H_{T, 2}$ values, the fraction arising from 2,3 -jet events remains close to $65 \%$ stressing once more the lower sensitivity of $H_{T, 2}$ versus $H_{T}$ regarding multiple jet production.

Finally, we compare the plots from the combined BHS samples in all figures to the corresponding ones generated with the $S$-MEPS sample. Interestingly, the outcome looks very similar although ME\&TS handles the single terms in Eq. (105) rather differently. They are calculated at least at leading (soft/collinear) logarithmic accuracy improved by LO $n$-jet effects. Presumably, for the exclusive jet bins, this description (which allows a better treatment of jet vetoes) is not too far off the exclusive sums


Fig. 59: Average number of jets as a function of $H_{T}$ (left) and $\Delta y$ (right) in two BHS descriptions, from $H E J$ and from $S$-MEPS, the latter using the $\langle N\rangle_{7}$ definition. The bands shown with dotted lines for the HEJ prediction are a result of varying the scale by a factor of 2 in each direction.
approach, since the unresolved $\mathcal{O}\left(\alpha_{s}\right)$ corrections are also present in the Sudakov form factors applied in the ME\&TS approach. Also, the combined BHS samples as well as the $S$-MEPS sample use the same tree-level matrix elements, namely up to $W+5$-parton matrix elements. Clearly, it has to be studied further whether this similarity in the results is a coincidence or not.

It is clear that the impact of the higher multiplicity samples is significant throughout, especially in the high $H_{T}$ tail. This is precisely the region, which would be probed for signs of new physics, and therefore it is essential that we fully understand our theoretical descriptions in this region. This is the subject of the remainder of this contribution, where we compare all four different methods of modelling hard QCD radiation in inclusive $W+2$-jet events.

The left plot of Fig. 59 shows the final comparison plot between the exclusive sums and inclusive 2-jet $B H S$ results as well as the $H E J$ and $S-M E P S$ predictions for the average number of jets as a function of $H_{T}$. The differences in the descriptions are significantly larger than the scale uncertainty band on the $H E J$ prediction. For the $W+2$-jet NLO result, the number of jets rises to 2.6 already at $H_{T}=500 \mathrm{GeV}$ but that levels off significantly below the $S-M E P S$, exclusive $B H S$ sum and $H E J$ results. The $H E J$ results level off at a higher value of about 3.0 , starting to clearly disagree with the exclusive sums and $S$-MEPS predictions above 500 GeV , from where those two curves keep rising to a final level of around 3.7 to 4.0. The $S$-MEPS comes in highest at largest $H_{T}$, where $\langle N\rangle_{7}$ is shown, cf. Eq. (106), in order to determine the average number of jets for this $S$-MEPS result. The reason for giving slightly higher $\langle N\rangle$ than the exclusive sums lies in the contribution of additional parton-shower jets present in the $S$-MEPS calculation and more accurately accounted for by the use of the $\langle N\rangle_{7}$ definition as compared to the earlier result based on $\langle N\rangle_{5}$ presented in Fig. 57 to the lower left.

In the right panel of Fig. 59, we have plotted the average number of jets as a function of the rapidity span, $\Delta y$, instead of $H_{T}$ as before. Again the differences are larger than the scale variation shown on the HEJ result, but the ordering is different to that of the left plot of Fig. 59. All four descriptions increase linearly with $\Delta y$ but the gradient is steepest for the HEJ predictions where the average rises above 3.0 for $\Delta y$ values as large as 6.0. The BHS exclusive sum result is consistently below this, reaching about 2.8 at $\Delta y=6.0$, and agrees pretty well with the $S$-MEPS result based on $\langle N\rangle_{7}$. The NLO $W+2$-jet prediction given by $B H S$ is lower still, between 2.4 and 2.5 for $\Delta y \sim 5.0$.

It may seem surprising that on the plot on the left-hand side the exclusive sums and S-MEPS lie higher for most of the distribution whereas on the right-hand side these approaches as well as $H E J$ give predicitions that are commensurate. The region of high $H_{T}$ and that of high $\Delta y$ however are largely distinct as it is very expensive to have both a large rapidity and large $p_{T}$ for the jets. Also while radiating


Fig. 60: The ratio of the inclusive 3 -jet and 2 -jet rates in the inclusive $W+2$-jet NLO and exclusive sum description of $B H S$ as well as in the $S$-MEPS and $H E J$ approaches as a function of $H_{T}$ (left) and $\Delta y$ (right). Again, the dotted lines indicate the uncertainty band from varying the scale in $H E J$ by a factor of 2 in each direction.
an additional jet automatically moves an event towards the higher $H_{T}$ direction, radiating an additional jet tends to not change the rapidity difference. So, we expect the higher multiplicies to have a smaller effect on the average number of jets as a function of $\Delta y$ compared to as a function of $H_{T}$. This is indeed the case in Fig. 59.

Lastly, in Fig. 60 we plot the ratio of the inclusive 3 -jet to the inclusive 2 -jet rate as a function of $H_{T}$ (left) and $\Delta y$ (right), again for all four descriptions used here. The predicted $\left(d \sigma_{3}^{\text {inc }} / d H_{T}\right) /\left(d \sigma_{2}^{\text {inc }} / d H_{T}\right)$ all agree very well below 400 GeV . The fixed order $B H S$ result for $W+2$ jets is highest for large $H_{T}$, however is known to become unreliable here, since the probability that an inclusive 2 -jet event is at least a 3 -jet event turns too large, being in conflict with the expected behaviour of an $\mathcal{O}\left(\alpha_{s}\right)$ correction. The BHS exclusive sums, the S-MEPS and the HEJ results, in this order, level off considerably lower with the HEJ fraction staying below $60 \%$ to $70 \%$, which leaves the other predictions again above the $H E J$ uncertainty envelope. In contrast, when the same ratio of jet rates is plotted against $\Delta y$, the $H E J$ prediction is consistently higher throughout. This again emphasises that differences in the descriptions come to light in different kinematic regions. However, in both cases here the magnitude of the differences is relatively small and would be rather difficult to distinguish in present experimental data.

### 17.4 CONCLUSIONS

We have compared a number of theoretical descriptions of $W^{-}$production in association with at least two jets. After outlining one possible method of combining NLO calculations of different multiplicities, we compared this with a pure NLO calculation of $W+2$-jets production obtained by BLACKHAT+SHERPA, a sample of leading-order events merged using the ME\&TS method of SHERPA, and the high-energy resummation of the HEJ framework.

We studied the average number of jets and the ratio of the 3 -jet and 2 -jet inclusive cross sections as a function of $\Delta y$ and of $H_{T}$. We find, with these simple cuts, some clear differences in the predictions when we study the average number of jets as a function of both $\Delta y$ and $H_{T}$. Smaller differences, which would be more difficult to disentangle experimentally, are found when we study the ratio of inclusive rates.

It would be very valuable to have an experimental study, which probed the average number of jets in $W$ production in association with at least two jets, to test our different descriptions of these important Standard Model processes.

## Tune comparisons

Deviation metrics per gen/tune and observable group:

| Gen | Tune | UE | Dijets | Multijets | Jet shapes | W and Z | Fragmentation | B frag |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AlpGen | HERWIG6 | - | 1.83 | 5.36 | 2.48 | 0.91 | - | - |
|  | PYTHIA6-AMBT1 | - | 1.55 | 2.80 | 0.61 | 0.53 | - | - |
|  | PYTHIA6-D6T | - | 1.38 | 2.67 | 2.31 | 1.67 | - | - |
|  | PYTHIA6-P2010 | - | 1.09 | 2.65 | 2.03 | 1.48 | - | - |
|  | PYTHIA6-P2011 | - | 1.12 | 2.60 | 0.48 | 0.24 | - | - |
|  | PYTHIA6-Z2 | - | 1.48 | 2.63 | 0.55 | 0.48 | - | - |
|  | PYTHIA6-profQ2 | - | 1.16 | 2.65 | 1.43 | 1.29 | - | - |
| HERWIG | AUET2-CTEQ6L1 | 0.43 | 0.55 | 0.77 | 0.35 | 0.58 | 22.80 | 2.38 |
|  | AUET2-LOxx | 0.25 | 0.71 | 0.60 | 0.39 | 0.88 | 22.13 | 2.29 |
| Herwig++ | 2.5.1-UE-EE-3-CTEQ6L1 | 0.27 | 0.87 | 0.78 | 0.51 | 0.98 | 10.58 | 1.32 |
|  | 2.5.1-UE-EE-3-MRSTLOxx | 0.23 | 1.05 | 0.78 | 0.50 | 0.65 | 10.58 | 1.32 |
| PYTHIA6 | AMBT1 | 0.39 | 1.20 | 0.54 | 0.77 | 0.27 | 0.93 | 1.65 |
|  | AUET2B-CTEQ6L1 | 0.16 | 0.92 | 0.44 | 0.59 | 0.74 | 0.67 | 1.29 |
|  | AUET2B-LOxx | 0.13 | 1.33 | 0.55 | 0.58 | 1.15 | 0.67 | 1.30 |
|  | D6T | 0.58 | 0.79 | 0.50 | 0.56 | 1.25 | 0.36 | 2.63 |
|  | DW | 0.81 | 0.78 | 0.61 | 0.56 | 1.33 | 0.36 | 2.63 |
|  | P2010 | 0.30 | 0.93 | 0.82 | 1.07 | 0.30 | 0.44 | 1.75 |
|  | P2011 | 0.12 | 0.89 | 0.67 | 1.02 | 0.53 | 0.43 | 2.13 |
|  | ProfQ2 | 0.51 | 0.67 | 0.81 | 0.51 | 0.64 | 0.30 | 1.65 |
|  | Z2 | 0.18 | 0.94 | 0.73 | 0.80 | 0.30 | 0.95 | 2.78 |
| Pythias | 4 C | 0.30 | 0.97 | 0.93 | 0.50 | 0.90 | 0.38 | 1.12 |
| Sherpa | 1.3.1 | 0.68 | 0.47 | 0.34 | 0.71 | 0.36 | 0.75 | 2.48 |

Fig. 111: Screenshot of the top-level summary page produced by the tune comparison system.
Jet shapes

| Histo | chi2/Nat | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Jet shape svinos for Sp_\.... (ATLAS_2011_S8924791/d01-x06-y01) | 0.59 | 0.77 | 0.69 | 1.17 | 0.77 |
| jet shape Svihos for Sp_lp... (ATLAS_2011_58924791/d09-×06-y01) | 0.14 | 0.36 | 0.30 | 0.61 | 0.36 |
| Central Transv. Thrust, $59 \ldots$ (CMS_2011_ $58957746 / 101 \times \times 01$-y01) | 0.37 | 0.43 | 0.53 | 1.08 | 0.53 |
| Central Transv. Minor, 590... (CMS_2011_58957746/d02-x01-y01) | 0.34 | 0.38 | 0.48 | 1.14 | 0.48 |

## W and Z

| Histo | chi2/Ndf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Muon channel ( $\mathrm{s} \mid \mathrm{y}$ _ $\mathrm{Z} \mid<1 \mathrm{~s}$ ) (D0_2010_ $58821313 / 802$-x01-y01) | 0.77 | 0.70 | 0.79 | 1.52 | 0.79 |
| Muon channel ( $\$ 1<\mid y \mathrm{z}$ Z\|<2s) (00_2010_s8821313/d02-x01-y02) | 0.27 | 0.38 | 0.45 | 1.08 | 0.45 |

## Fragmentation

| Histo | chi2/Wdf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Scaled momentum, 5x.p = \|p... (DELPH1_1996_S3430090/d07-x01-y01) | 0.74 | 0.28 | 0.47 | 3.29 | 0.47 |
| S1-text(Thrust)s (DELPHI_1996_S3430090/d11-x01-y01) | 4.12 | 0.24 | 1.13 | 8.26 | 1.13 |
| Thrust major, SMS (DELPH1_1996_53430090/d12-x01-y01) | 7.24 | 0.50 | 1.61 | 9.37 | 1.61 |
| Thrust minor, sms (DELPH1_1996_53430090/d13-x01-y01) | 9.69 | 0.40 | 1.57 | 10.58 | 10.58 |
| Mean charged mutitilicity (DELPH1_1996_S3430090/d35-x01-y01) | 0.08 | 0.28 | 0.28 | 0.28 | 0.28 |

Fig. 112: Screenshot of the mid-level performance metric page produced by the tune comparison system. This specific example is part of the performance metrics for the Herwig++ LHC-UE-EE-3 LO $* *$ tune.

FFNS for small $Q$, and the ZM-VFNS for large $Q$. In Fig. $2(\mathrm{~b})$, we plot $F_{2}^{c}$ as a function of the quark mass $m$ for a fixed $Q=10 \mathrm{GeV}$ for the MS ZM-VFNS and ACOT schemes. We observe that when $m$ is within a decade or two of $\mu$, the quark mass plays a dynamic role; however, for $m \ll \mu$, the quark mass purely serves as a regulator and the specific value is not important. Operationally, it means we can obtain the $\overline{\mathrm{MS}} \mathrm{ZM}-V F N S$ result either by (i) computing the terms using dimensional regularization and setting the regulator to zero, or (ii) by computing the terms using the quark mass as the regulator and then setting this to zero.


Fig. 2. (a) $F_{2}^{c}$ for $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number Scheme (FFNS), and Zero-Mass Variable Flavor Number Scheme (ZM-VFNS). The ACOT and S-ACOT results are virtually identical. (b) Comparison of $F_{2}^{c}(x, Q)$ (scaled by $10^{4}$ ) vs. the quark mass $m$ in GeV for fixed $x=0.1$ and $Q=10 \mathrm{GeV}$. The full (red) dots are the full ACOT result, and the solid (blue) line is the massless $\overline{\mathrm{MS}}$ result.

The ACOT scheme is minimal in the sense that the construction of the massive short distance cross sections does not need any observabledependent extra contributions or any regulators to smooth the transition between the high and low scale regions. The ACOT prescription is: (a) calculate the massive partonic cross sections, and (b) perform the factorization using the quark mass as regulator.

It is in this sense that we claim the ACOT scheme is the minimal massive extension of the $\overline{\mathrm{MS}}$ ZM-VFNS. In the limit $m / \mu \rightarrow 0$ it reduces exactly to the $\overline{\mathrm{MS}} \mathrm{ZM}-V F N S$, in the limit $m / \mu \gtrsim 1$ the heavy quark decouples from the PDFs and we obtain exactly the FFNS for $m / \mu \gg 1$ and no finite renormalizations are needed.

### 2.2. S-ACOT

In a corresponding application, it was observed that the heavy quark mass could be set to zero in certain pieces of the hard scattering terms without any loss of accuracy. This modification of the ACOT scheme goes by the name Simplified-ACOT (S-ACOT) and can be summarized as follows [8].


Fig. 2: a) $F_{2}^{c}$ for $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number Scheme (FFNS), and Zero-Mass Variable Flavor Number Scheme (ZM-VFNS). The ACOT and S-ACOT results are virtually identical.
b) Comparison of $F_{2}^{c}(x, Q)$ (scaled by $10^{4}$ ) vs. the quark mass $m$ in GeV for fixed $x=0.1$ and $Q=10 \mathrm{GeV}$. The red dots are the full ACOT result, and the blue line is the massless $\overline{M S}$ result.

Operationally, it means we can obtain the $\overline{M S}$ ZM-VFNS result either by i) computing the terms using dimensional regularization and setting the regulator to zero, or ii) by computing the terms using the quark mass as the regulator and then setting this to zero.

The ACOT scheme is minimal in the sense that the construction of the massive short distance cross sections does not need any observabledependent extra contributions or any regulators to smooth the transition between the high and low scale regions. The ACOT prescription is: a) calculate the massive partonic cross sections, and b) perform the factorization using the quark mass as regulator.

It is in this sense that we claim the ACOT scheme is the minimal massive extension of the $\overline{M S}$ ZM-VFNS. In the limit $m / \mu \rightarrow 0$ it reduces exactly to the $\overline{M S}$ ZM-VFNS, in the limit $m / \mu \gtrsim 1$ the heavy quark decouples from the PDFs and we obtain exactly the FFNS for $m / \mu \gg 1$ and no finite renormalizations are needed.

## 2.2. $S$-ACOT

In a corresponding application, it was observed that the heavy quark mass could be set to zero in certain pieces of the hard scattering terms without any loss of accuracy. This modification of the ACOT scheme goes by the name Simplified-ACOT (S-ACOT) and can be summarized as follows [8].

S-ACOT: For hard-scattering processes with incoming heavy


Fig. 17: Example Feynman diagrams contributing to DIS heavy quark production (from left): LO $\mathcal{O}\left(\alpha_{S}^{0}\right)$ quark-boson scattering $Q V \rightarrow Q$, NLO $\mathcal{O}\left(\alpha_{S}^{1}\right)$ boson-gluon scattering $g V \rightarrow Q \bar{Q}$, NNLO $\mathcal{O}\left(\alpha_{S}^{2}\right)$ boson-gluon scattering $g V \rightarrow g Q \bar{Q}$ and $\mathrm{N}^{3} \mathrm{LO} \mathcal{O}\left(\alpha_{S}^{3}\right)$ boson-gluon scattering $g V \rightarrow g g Q \bar{Q}$.
prediction for $F_{L}$ is a challenge, particularly in the region of low $Q^{2}$ and small $x$.
In this paper, we will briefly outline the method we used to incorporate the higher order terms, the key elements of the ACOT scheme, and the treatment of the heavy quark masses. We then present results for the $F_{2}$ and $F_{L}$ neutral current DIS structure functions.

### 9.2 THE ACOT SCHEME AND ITS EXTENSION BEYOND NLO



Fig. 18: Comparison of schemes for $F_{2}^{c}$ at $x=0.1$ for NLO DIS heavy quark production as a function of $Q$. We display calculations using the ACOT, S-ACOT, Fixed-Flavor Number Scheme (FFNS), and Zero-Mass Variable-Flavor-Number-Scheme (ZM-VFNS). The ACOT and S-ACOT results are virtually identical.

The ACOT scheme [322, 323] is based upon the factorization theorem for heavy quarks[324]; hence, it is valid at any order of perturbation theory. The factorization proof ensures that the ACOT scheme can be applied throughout the full kinematic regime, and that there is a smooth transition from a massless result $(m=0)$ to the heavy-mass decoupling limit $(m \rightarrow \infty)$.

In the limit where the quark $Q$ of mass $m$ is relatively heavy compared to the characteristic energy scale ( $\mu \lesssim m$ ), the ACOT result naturally reduces to the Fixed-Flavor-Number-Scheme (FFNS). In the FFNS, the heavy quark is treated as being extrinsic to the hadron, and there is no corresponding heavy quark PDF, $f_{Q}(x, \mu)=0$. Conversely, in the limit where the quark mass is relatively light $(\mu \gtrsim m)$, the ACOT result reduces to the $\overline{M S}$ Zero-Mass Variable-Flavor-Number-Scheme (ZM-VFNS) exactlywithout any finite renormalizations. In this limit, the quark mass $m$ no longer plays any dynamical role; it serves purely as a regulator. This feature is presented in Fig. 18 where we can see that the ACOT scheme precisely matches the results of the FFNS and ZM-VFNS schemes in their respective limits.

Additionally Fig. 18 shows the results obtained within the Simplified-ACOT scheme (SACOT) [325]. The S-ACOT scheme drops the heavy quark mass dependence for the hard-scattering

$$
\begin{array}{ll}
\left|\eta_{e}\right|<2.5 & p_{T, e}>20 \mathrm{GeV} \\
M_{\perp, W}>20 \mathrm{GeV} & p_{T, \nu}>20 \mathrm{GeV} \\
\left|\eta_{j}\right|<4.5 & p_{T, j}>25 \mathrm{GeV}
\end{array}
$$

Table 12: Summary of the cuts applied in the analysis.


Fig. 56: The average number of jets as a function of $p_{T, W}$ (left) and $p_{T, j_{1}}$ (right). The $p_{T, W}$ plot shows the $B H S$ exclusive sums prediction, while the $p_{T, j_{1}}$ plot is obtained from $S$-MEPS.

### 17.3 RESULTS OF THE COMPARISON

In this section, we compare the results of different theoretical descriptions for $W+n$-jets production at the LHC. The number $n$ can take values from 2 and above, as we will mostly consider inclusive samples. The four descriptions, which we will compare here in more detail, are

- the $B H S$ calculation of $W+2$-jets at NLO,
- the combined sample of $W+2,3,4$-jet events at NLO from $B H S$, as described in the 17.2 section,
- the $S$-MEPS merged $W+n$-jets sample using LO tree-level matrix elements up to $n=5$, and
- the approach of $H E J$.

Throughout this study, we will consider inclusive samples of $W^{-}$boson production in association with at least two hard jets identified by the anti- $k_{T}$ jet algorithm using $R=0.4$. The jets are required to have $p_{T, j}>25 \mathrm{GeV}$. We look only in the $W^{-} \rightarrow e^{-} \bar{\nu}_{e}$ decay channel and use the cuts given in Tab. 12 where $M_{\perp, W}$ is defined as $M_{\perp, W}=\sqrt{\left(\left|\vec{p}_{T, e}\right|+\left|\vec{p}_{T, \nu}\right|\right)^{2}-\left(\vec{p}_{T, e}+\vec{p}_{T, \nu}\right)^{2}}$.

The HEJ predictions use the geometric mean of the jet transverse momenta to determine the renormalisation and factorisation scale, i.e. $\left(\prod p_{T, j}\right)^{1 / n}$. This central choice will be varied by a factor of two in either direction to provide an envelope (marked by dotted lines in the corresponding figures) around the HEJ default prediction. The BHS predictions instead use $\hat{H}_{T}^{\prime} / 2$ as the NLO calculation becomes unstable for a scale which is too low. In the $S$-MEPS calculation, scales are chosen according to the default prescription given by ME\&TS [426].

The variables $H_{T, 2}, p_{T, W}$ and $p_{T, j_{1}}$ are less sensitive to the presence of additional radiation than $H_{T}$, as discussed in the introduction. The plots, which we present in Figs. 56 and 57 address the alternative question: given a particular value of $H_{T}, H_{T, 2}$ etc. how many jets are typically found in the event?

Figs. 56 and 57 show the stacked results for the average number of jets as a function of $p_{T, W}, p_{T, j_{1}}$, $H_{T}$ and $H_{T, 2}$ visualising the contributions from each exclusive 2,3,4-jet sample and the inclusive 5 -jet


Fig. 57: The contribution from different multiplicities to the average number of jets as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the BHS exclusive sums prediction, while the lower ones are extracted from S-MEPS.
sample. The left (right) plot in Fig. 56 and the upper (lower) rows of plots in Fig. 57 depict the results as obtained from the combined BHS sample (the $S$-MEPS sample). In all cases the different colours correspond to the terms in the numerator of the formula for the average number of jets,

$$
\begin{equation*}
\langle N\rangle_{5}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}=\frac{\sum_{i=2,3,4} i n_{i}^{\mathrm{exc}}+5 n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{106}
\end{equation*}
$$

where blue, green, red and magenta stand for $i=2,3,4$ and $i=5$, respectively. The subscript to $\langle N\rangle$ clarifies that we truncate the determination of the average after the fifth jet bin, noting that $\langle N\rangle_{k} \rightarrow\langle N\rangle$ for a sufficiently large number of jet bins. This makes no difference for the BHS predictions employed here since the jet multiplicity de facto is limited to five, but it does for the $S$-MEPS and HEJ computations where events with $i>5$ jets do occur. We have defined $n_{k}^{\text {exc } / \mathrm{inc}}=d \sigma_{k}^{\text {exc } / \mathrm{inc}} / d O$ where $O$ denotes an observable like $H_{T}$, or $\Delta y$ presented later on. Note that in Fig. 57 the 5 -jet part contributes to the average number of jets with a factor of 5 , while the 2 -jet part, for example, contributes with a factor of 2 only.

The layout of Fig. 58 (including the colour coding) is the same as before: here, we however display, wrt. $n_{2}^{\text {inc }}$, the relative fractions of the different multiplicities corresponding to the terms in the denominator of Eq. (106). In other words, in Fig. 58 we consider the partitioning of

$$
\begin{equation*}
1=\frac{\sum_{i=2,3,4} n_{i}^{\mathrm{exc}}+n_{5}^{\mathrm{inc}}}{n_{2}^{\mathrm{inc}}} \tag{107}
\end{equation*}
$$



Fig. 58: The fraction of the total rate from different multiplicities as a function of $H_{T}$ and $H_{T, 2}$. The upper plots show the $B H S$ exclusive sums prediction, while the lower ones are extracted from $S$-MEPS.

Although there is just a $30 \%$ fraction of inclusive 5 -jet events to the total cross section, we observe that their contribution to the build-up of $\langle N\rangle\left(H_{T}\right)$ for very large $H_{T}$ gets close to $50 \%$. Also, for an $H_{T} \sim$ 500 GeV , the average number of jets is composed evenly between the 2,3 -jet and 4,5 -jet contributions, while the relative fraction of the 2,3 -jet events is nearly $70 \%$. This emphasizes the dominance of multijet events in forming large $H_{T}$ values. It also can be seen that for medium $H_{T}$ values, $400<H_{T}<$ 700 GeV , all the multiplicities give roughly the same contribution to the variable $\langle N\rangle\left(H_{T}\right)$, while for low $H_{T}$, the average is primarily described by 2-jet events.

Going clockwise through Figs. 56 and 57 we see that the average number of jets is indeed sensitive to higher multiplicities when considered as a function of $p_{T, W}, p_{T, j_{1}}$ and $H_{T, 2}$, but in all these cases this happens to a lesser extent as if considered as a function of $H_{T}$. As expected, the dependence is mildest for $p_{T, W}$, the most inclusive observable studied here. We also observe that the jet-bin decomposition of $p_{T, j_{1}}$ and $H_{T, 2}$ turns out very similar. Most strikingly we note the increase in the contribution from the highest multiplicity events, the ones containing more or at least five jets. For $H_{T, 2}$, we furthermore display to the right of Fig. 58 the relative fractions as done in the $H_{T}$ case. Even for largest $H_{T, 2}$ values, the fraction arising from 2,3 -jet events remains close to $65 \%$ stressing once more the lower sensitivity of $H_{T, 2}$ versus $H_{T}$ regarding multiple jet production.

Finally, we compare the plots from the combined BHS samples in all figures to the corresponding ones generated with the $S$-MEPS sample. Interestingly, the outcome looks very similar although ME\&TS handles the single terms in Eq. (105) rather differently. They are calculated at least at leading (soft/collinear) logarithmic accuracy improved by LO $n$-jet effects. Presumably, for the exclusive jet bins, this description (which allows a better treatment of jet vetoes) is not too far off the exclusive sums


Fig. 59: Average number of jets as a function of $H_{T}$ (left) and $\Delta y$ (right) in two BHS descriptions, from $H E J$ and from $S$-MEPS, the latter using the $\langle N\rangle_{7}$ definition. The bands shown with dotted lines for the HEJ prediction are a result of varying the scale by a factor of 2 in each direction.
approach, since the unresolved $\mathcal{O}\left(\alpha_{s}\right)$ corrections are also present in the Sudakov form factors applied in the ME\&TS approach. Also, the combined BHS samples as well as the $S$-MEPS sample use the same tree-level matrix elements, namely up to $W+5$-parton matrix elements. Clearly, it has to be studied further whether this similarity in the results is a coincidence or not.

It is clear that the impact of the higher multiplicity samples is significant throughout, especially in the high $H_{T}$ tail. This is precisely the region, which would be probed for signs of new physics, and therefore it is essential that we fully understand our theoretical descriptions in this region. This is the subject of the remainder of this contribution, where we compare all four different methods of modelling hard QCD radiation in inclusive $W+2$-jet events.

The left plot of Fig. 59 shows the final comparison plot between the exclusive sums and inclusive 2-jet $B H S$ results as well as the $H E J$ and $S-M E P S$ predictions for the average number of jets as a function of $H_{T}$. The differences in the descriptions are significantly larger than the scale uncertainty band on the $H E J$ prediction. For the $W+2$-jet NLO result, the number of jets rises to 2.6 already at $H_{T}=500 \mathrm{GeV}$ but that levels off significantly below the $S-M E P S$, exclusive $B H S$ sum and $H E J$ results. The $H E J$ results level off at a higher value of about 3.0 , starting to clearly disagree with the exclusive sums and $S$-MEPS predictions above 500 GeV , from where those two curves keep rising to a final level of around 3.7 to 4.0. The $S$-MEPS comes in highest at largest $H_{T}$, where $\langle N\rangle_{7}$ is shown, cf. Eq. (106), in order to determine the average number of jets for this $S$-MEPS result. The reason for giving slightly higher $\langle N\rangle$ than the exclusive sums lies in the contribution of additional parton-shower jets present in the $S$-MEPS calculation and more accurately accounted for by the use of the $\langle N\rangle_{7}$ definition as compared to the earlier result based on $\langle N\rangle_{5}$ presented in Fig. 57 to the lower left.

In the right panel of Fig. 59, we have plotted the average number of jets as a function of the rapidity span, $\Delta y$, instead of $H_{T}$ as before. Again the differences are larger than the scale variation shown on the HEJ result, but the ordering is different to that of the left plot of Fig. 59. All four descriptions increase linearly with $\Delta y$ but the gradient is steepest for the HEJ predictions where the average rises above 3.0 for $\Delta y$ values as large as 6.0. The BHS exclusive sum result is consistently below this, reaching about 2.8 at $\Delta y=6.0$, and agrees pretty well with the $S$-MEPS result based on $\langle N\rangle_{7}$. The NLO $W+2$-jet prediction given by $B H S$ is lower still, between 2.4 and 2.5 for $\Delta y \sim 5.0$.

It may seem surprising that on the plot on the left-hand side the exclusive sums and S-MEPS lie higher for most of the distribution whereas on the right-hand side these approaches as well as $H E J$ give predicitions that are commensurate. The region of high $H_{T}$ and that of high $\Delta y$ however are largely distinct as it is very expensive to have both a large rapidity and large $p_{T}$ for the jets. Also while radiating


Fig. 60: The ratio of the inclusive 3 -jet and 2 -jet rates in the inclusive $W+2$-jet NLO and exclusive sum description of $B H S$ as well as in the $S$-MEPS and $H E J$ approaches as a function of $H_{T}$ (left) and $\Delta y$ (right). Again, the dotted lines indicate the uncertainty band from varying the scale in $H E J$ by a factor of 2 in each direction.
an additional jet automatically moves an event towards the higher $H_{T}$ direction, radiating an additional jet tends to not change the rapidity difference. So, we expect the higher multiplicies to have a smaller effect on the average number of jets as a function of $\Delta y$ compared to as a function of $H_{T}$. This is indeed the case in Fig. 59.

Lastly, in Fig. 60 we plot the ratio of the inclusive 3 -jet to the inclusive 2 -jet rate as a function of $H_{T}$ (left) and $\Delta y$ (right), again for all four descriptions used here. The predicted $\left(d \sigma_{3}^{\text {inc }} / d H_{T}\right) /\left(d \sigma_{2}^{\text {inc }} / d H_{T}\right)$ all agree very well below 400 GeV . The fixed order $B H S$ result for $W+2$ jets is highest for large $H_{T}$, however is known to become unreliable here, since the probability that an inclusive 2 -jet event is at least a 3 -jet event turns too large, being in conflict with the expected behaviour of an $\mathcal{O}\left(\alpha_{s}\right)$ correction. The BHS exclusive sums, the S-MEPS and the HEJ results, in this order, level off considerably lower with the HEJ fraction staying below $60 \%$ to $70 \%$, which leaves the other predictions again above the $H E J$ uncertainty envelope. In contrast, when the same ratio of jet rates is plotted against $\Delta y$, the $H E J$ prediction is consistently higher throughout. This again emphasises that differences in the descriptions come to light in different kinematic regions. However, in both cases here the magnitude of the differences is relatively small and would be rather difficult to distinguish in present experimental data.

### 17.4 CONCLUSIONS

We have compared a number of theoretical descriptions of $W^{-}$production in association with at least two jets. After outlining one possible method of combining NLO calculations of different multiplicities, we compared this with a pure NLO calculation of $W+2$-jets production obtained by BLACKHAT+SHERPA, a sample of leading-order events merged using the ME\&TS method of SHERPA, and the high-energy resummation of the HEJ framework.

We studied the average number of jets and the ratio of the 3 -jet and 2 -jet inclusive cross sections as a function of $\Delta y$ and of $H_{T}$. We find, with these simple cuts, some clear differences in the predictions when we study the average number of jets as a function of both $\Delta y$ and $H_{T}$. Smaller differences, which would be more difficult to disentangle experimentally, are found when we study the ratio of inclusive rates.

It would be very valuable to have an experimental study, which probed the average number of jets in $W$ production in association with at least two jets, to test our different descriptions of these important Standard Model processes.

## Tune comparisons

Deviation metrics per gen/tune and observable group:

| Gen | Tune | UE | Dijets | Multijets | Jet shapes | W and Z | Fragmentation | B frag |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| AlpGen | HERWIG6 | - | 1.83 | 5.36 | 2.48 | 0.91 | - | - |
|  | PYTHIA6-AMBT1 | - | 1.55 | 2.80 | 0.61 | 0.53 | - | - |
|  | PYTHIA6-D6T | - | 1.38 | 2.67 | 2.31 | 1.67 | - | - |
|  | PYTHIA6-P2010 | - | 1.09 | 2.65 | 2.03 | 1.48 | - | - |
|  | PYTHIA6-P2011 | - | 1.12 | 2.60 | 0.48 | 0.24 | - | - |
|  | PYTHIA6-Z2 | - | 1.48 | 2.63 | 0.55 | 0.48 | - | - |
|  | PYTHIA6-profQ2 | - | 1.16 | 2.65 | 1.43 | 1.29 | - | - |
| HERWIG | AUET2-CTEQ6L1 | 0.43 | 0.55 | 0.77 | 0.35 | 0.58 | 22.80 | 2.38 |
|  | AUET2-LOxx | 0.25 | 0.71 | 0.60 | 0.39 | 0.88 | 22.13 | 2.29 |
| Herwig++ | 2.5.1-UE-EE-3-CTEQ6L1 | 0.27 | 0.87 | 0.78 | 0.51 | 0.98 | 10.58 | 1.32 |
|  | 2.5.1-UE-EE-3-MRSTLOxx | 0.23 | 1.05 | 0.78 | 0.50 | 0.65 | 10.58 | 1.32 |
| PYTHIA6 | AMBT1 | 0.39 | 1.20 | 0.54 | 0.77 | 0.27 | 0.93 | 1.65 |
|  | AUET2B-CTEQ6L1 | 0.16 | 0.92 | 0.44 | 0.59 | 0.74 | 0.67 | 1.29 |
|  | AUET2B-LOxx | 0.13 | 1.33 | 0.55 | 0.58 | 1.15 | 0.67 | 1.30 |
|  | D6T | 0.58 | 0.79 | 0.50 | 0.56 | 1.25 | 0.36 | 2.63 |
|  | DW | 0.81 | 0.78 | 0.61 | 0.56 | 1.33 | 0.36 | 2.63 |
|  | P2010 | 0.30 | 0.93 | 0.82 | 1.07 | 0.30 | 0.44 | 1.75 |
|  | P2011 | 0.12 | 0.89 | 0.67 | 1.02 | 0.53 | 0.43 | 2.13 |
|  | ProfQ2 | 0.51 | 0.67 | 0.81 | 0.51 | 0.64 | 0.30 | 1.65 |
|  | Z2 | 0.18 | 0.94 | 0.73 | 0.80 | 0.30 | 0.95 | 2.78 |
| Pythias | 4 C | 0.30 | 0.97 | 0.93 | 0.50 | 0.90 | 0.38 | 1.12 |
| Sherpa | 1.3.1 | 0.68 | 0.47 | 0.34 | 0.71 | 0.36 | 0.75 | 2.48 |

Fig. 111: Screenshot of the top-level summary page produced by the tune comparison system.
Jet shapes

| Histo | chi2/Nat | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Jet shape svinos for Sp_\.... (ATLAS_2011_S8924791/d01-x06-y01) | 0.59 | 0.77 | 0.69 | 1.17 | 0.77 |
| jet shape Svihos for Sp_lp... (ATLAS_2011_58924791/d09-×06-y01) | 0.14 | 0.36 | 0.30 | 0.61 | 0.36 |
| Central Transv. Thrust, $59 \ldots$ (CMS_2011_ $58957746 / 101 \times \times 01$-y01) | 0.37 | 0.43 | 0.53 | 1.08 | 0.53 |
| Central Transv. Minor, 590... (CMS_2011_58957746/d02-x01-y01) | 0.34 | 0.38 | 0.48 | 1.14 | 0.48 |

## W and Z

| Histo | chi2/Ndf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Muon channel ( $\mathrm{s} \mid \mathrm{y}$ _ $\mathrm{Z} \mid<1 \mathrm{~s}$ ) (D0_2010_ $58821313 / 802$-x01-y01) | 0.77 | 0.70 | 0.79 | 1.52 | 0.79 |
| Muon channel ( $\$ 1<\mid y \mathrm{z}$ Z\|<2s) (00_2010_s8821313/d02-x01-y02) | 0.27 | 0.38 | 0.45 | 1.08 | 0.45 |

## Fragmentation

| Histo | chi2/Wdf | Median deviation | Mean deviation | Max deviation | Metric |
| :---: | :---: | :---: | :---: | :---: | :---: |
| Scaled momentum, 5x.p = \|p... (DELPH1_1996_S3430090/d07-x01-y01) | 0.74 | 0.28 | 0.47 | 3.29 | 0.47 |
| S1-text(Thrust)s (DELPHI_1996_S3430090/d11-x01-y01) | 4.12 | 0.24 | 1.13 | 8.26 | 1.13 |
| Thrust major, SMS (DELPH1_1996_53430090/d12-x01-y01) | 7.24 | 0.50 | 1.61 | 9.37 | 1.61 |
| Thrust minor, sms (DELPH1_1996_53430090/d13-x01-y01) | 9.69 | 0.40 | 1.57 | 10.58 | 10.58 |
| Mean charged mutitilicity (DELPH1_1996_S3430090/d35-x01-y01) | 0.08 | 0.28 | 0.28 | 0.28 | 0.28 |

Fig. 112: Screenshot of the mid-level performance metric page produced by the tune comparison system. This specific example is part of the performance metrics for the Herwig++ LHC-UE-EE-3 LO $* *$ tune.
parametrize the nPDFs at the initial $Q_{0}^{2}=1 \mathrm{GeV}^{2}$ using Eq. (5.134) and

$$
\begin{equation*}
R_{i}\left(x_{B}, Q_{0}^{2}, A, Z\right)=1+\left(1-\frac{1}{A^{\alpha}}\right) \frac{a_{i}+b_{i} x+c_{i} x^{2}+d_{i} x^{3}}{(1-x)^{\beta_{i}}} \tag{5.135}
\end{equation*}
$$

The determined $u_{v}, \bar{q}$, and $g$ nPDFs from the HKN07 analysis [38] are shown for the calcium nucleus in Fig. 5.55 at $Q^{2}=1 \mathrm{GeV}^{2}$. LO and NLO results are shown with uncertainty bands, showing that nPDFs are determined more accurately at NLO. We obtain $\chi_{\text {min }}^{2} /$ d.o.f. $=1.35$ and 1.21 for the LO and NLO fits, respectively.

The valence-quark modifications are well determined because of accurate measurements on the $F_{2}$ ratios at medium $x$. The small- $x$ region is fixed by the baryon-number and charge conservations together with the modifications in the medium- and large- $x$ regions. The antiquark modifications are also determined well at small $x$ due to measurements on $F_{2}$ shadowing, and they are also fixed at $x \sim 0.1$ because of Fermilab Drell-Yan measurements. However, the region at $x>0.2$ is not determined at all. The E906/SeaQuest collaboration is currently measuring this medium- $x$ region, and there is also a possibility to measure this region with an experiment at J-PARC. In the near future, the uncertainty bands should be significantly reduced for the antiquark.

The gluon distribution has the largest uncertainties since it contributes to the $F_{2}$ and Drell-Yan ratios only as higher-order effects, and the $Q^{2}$ dependence of $F_{2}^{A} / F_{2}^{A^{\prime}}$ is not measured accurately on nuclear targets, which makes it difficult to pin down the gluon modifications measured by scaling violations of $F_{2}$. The small- $x$ nPDFs are dominated by huge gluon distributions, so that it is essential to determine them accurately for new discoveries by high-energy heavyion experiments. Therefore, it is important to mea-


Figure 5.55. Determined nuclear modifications in Ca [38]. sure the $Q^{2}$ dependence of $F_{2}^{A} / F_{2}^{A^{\prime}}$ at EIC for determining nuclear gluon distributions.

In HKN07, the nPDFs are also investigated for the deuteron. In obtaining the "nucleonic" PDFs, deuteron data are used after crude nuclear corrections. Since the current PDFs could possibly contain nuclear effects, appropriate nuclear corrections should be applied in future for excluding such effects. Our codes for calculating the nPDFs and their uncertainties are available at the web site [970]. The technical details are explained in Refs. $[965,38]$ and within the subroutine.


FIG. 14: Shifts in $g_{L}^{2}$ and $g_{R}^{2}$ due to leptoquarks. Horizontal lines indicate the projected $1 \sigma$ limits of NuSOnG.


FIG. 15: NuSOnG expectation in the case of a Tev-scale triplet leptoquark. For clarity, this plot and the two following cases, show the expectation from only the two highest precision measurements from NuSOnG: $g_{L}^{2}$ and $\nu$ ES.
violation explains the NuTeV anomaly, thus the NuTeV PW and the NuSOnG PW measurements agree with the $\nu$ eES measurements. These three precision neutrino results, all with "LEP-size" errors, can be combined and will intersect the one-sigma edge of the LEP measurements. Fig. 16 illustrates this example. From this, the source, a fourth generation with isospin violation, can be


FIG. 16: NuSOnG expectation if the NuTeV anomaly is due to isospin violation and there is a heavy 4th generation with isospin violation.


FIG. 17: If LHC sees a Standard Model Higgs and no evidence of new physics, NuSOnG may reveal new physics in the neutrino sector.
demonstrated.
Lastly, while it seems unlikely, it is possible that LHC will observe a Standard Model Higgs and no signatures of new physics. If this is the case, it is still possible for NuSOnG to add valuable clues to new physics. This is because the experiment is uniquely sensitive to the neutrino sector. If a situation such as is illustrated on Fig. 17 arose, the only explanation would be new physics unique to neutrino interactions.

## VI. SUMMARY AND CONCLUSIONS

NuSOnG is an experiment which can search for new physics from keV through TeV energy scales, as well as make interesting QCD measurements. This article has focussed mainly on the Terascale physics which can be accessed through this new high energy, high statistics


Figure 3: Three projected electroweak measurements from NuSOnG in S-T plane. LEP/SLD error ellipse is shown in red and the current $\mathrm{NuTeV} \nu-q$ measurement is shown as a light blue band. The ochre band shows NuSOnG $\bar{\nu}-e$, the dark blue band shows NuSOnG $\nu-q$ and the green shows NuSOnG $\nu-e$. The width of the bands correspond to $68 \%$ confidence level for statistics as described in the text. The NuSOnG measurements assume $(S, T)=(0,0)$.
sensitive to new physics that violates isospin and is zero for new physics that conserves isospin. Isospin-breaking new physics such as heavy non-degenerate fermion doublets or scalar multiplets would affect the $T$ parameter. The $S$ parameter is sensitive to isospin-conserving physics, such as heavy degenerate fermion doublets.

The status of electroweak measurements are shown in Fig. 3 [8]. The combined analysis of the LEP and SLD data by the LEP Electroweak Working Group (EWWG) [9] indicates an allowed region shown by the small oval, centered at $S=0.05 \pm 0.10$ and $T=0.07 \pm 0.11$. A different choice of reference Higgs or top mass changes Standard Model predictions for observables and thus shifts the center of the $S T$ plot [10]; setting the Higgs mass to 1000 GeV would shift the center of the oval to roughly $(S, T)=$ $(0.12,-0.36)$. Measurements of the $W$ mass, which are not shown, are also consistent with the LEP measurements. The highest precision neutrino result comes from $\nu q$ and $\bar{\nu} q$ scattering by the NuTeV experiment. This result clearly disagrees with the other


Figure 6: Three projected electroweak measurements from NuSOnG in S-T plane for a model model with a heavy Higgs inspired by the NuTeV measurement [11]. In this model, $(S, T)=(0.12,-0.36)$. The labeling is as in Fig. 3.

## Hornbostel Publications

# Precise charm to strange mass ratio and light quark masses from full lattice QCD 

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#### Abstract

By using a single formalism to handle charm, strange and light valence quarks in full lattice QCD for the first time, we are able to determine ratios of quark masses to $1 \%$. For $m_{c} / m_{s}$ we obtain $11.85(16)$, an order of magnitude more precise than the current PDG average. Combined with $1 \%$ determinations of the charm quark mass now possible this gives $\bar{m}_{s}(2 \mathrm{GeV})=92.4(1.5) \mathrm{MeV}$. The MILC result for $m_{s} / m_{l}=27.2(3)$ yields $\bar{m}_{l}(2 \mathrm{GeV})=3.40(7) \mathrm{MeV}$ for the average of $u$ and $d$ quark masses.


Introduction. - The masses of $u, d$ and $s$ quarks are some of the least well-known parameters of the Standard Model. Even the most inaccurate lepton mass (that of the $\tau$ ) is known to better than $0.01 \%$ and yet errors on light quark masses of $30 \%$ are quoted in the Particle Data Tables [1]. The reason for the mismatch is the confinement property of the strong force that obscures the connection between the properties of the quark constituents and the hadron physics that is accessible to experiment. To make this connection requires accurate calculations in QCD and accurate experimental results for appropriate hadronic quantities. A method particularly well-suited to this is lattice QCD. Here we will demonstrate its use by determining $m_{c} / m_{s}$ to $1 \%$ and obtaining as a result $1.5 \%$ errors for light quark masses, which brings them almost into line with those of heavy quarks.

Heavy quark masses, $m_{Q}$, can be determined accurately because $\alpha_{s}\left(m_{Q}\right)$ is relatively small. $1 \%$ errors for charm and bottom quark masses have recently become possible using $\mathcal{O}\left(\alpha_{s}^{3}\right)$ calculations in QCD perturbation theory for the heavy quark vacuum 'bubble' [2] and therefore for the energy-derivative (or time) moments of correlation functions for a heavy quark-antiquark pair at zero momentum. Since the scale of $\alpha_{s}$ is naturally related to the relevant heavy quark mass, the expressions can be evaluated accurately. To extract the quark mass the perturbative result is compared to a nonperturbative determination containing information from experiment. For a $1^{--} Q \bar{Q}$ configuration moments of the experimentally measured cross-section for $\left(e^{+} e^{-} \rightarrow \gamma^{*} \rightarrow\right.$ hadrons $)$ can be used after isolating the heavy quark contribution and using dispersion relations [3]. Alternatively the time-moments for heavy quark current-current correlation functions of various $J^{P C}$ can be directly determined in lattice QCD calculations that have been tuned so that a charmonium or bottomonium mass agrees with experi-
ment [4, 5]. The time moments must be extrapolated to the zero lattice spacing (continuum) limit before the comparison to QCD perturbation theory. These two methods give results that agree, with $1 \%$ errors for $m_{c}(3 \mathrm{GeV})$ in the $\overline{M S}$ scheme. The more traditional 'direct' lattice QCD method, although somewhat less accurate, also gives results in good agreement [6. We can conclude from this that $m_{c}$ is now accurately known.

The strange quark mass, $m_{s}$, being much smaller, cannot be determined this way and is poorly known at present. Instead of a direct determination of $m_{s}$, however, we can use the leverage of an accurate result for the ratio $m_{c} / m_{s}$ combined with the accurate $m_{c}$ above [7]. But simple ratios of hadron mass differences give unreliable estimates of $m_{c} / m_{s}$. Two such estimates:

$$
\begin{equation*}
\frac{m\left(B_{c}\right)-m\left(B_{u}\right)}{m\left(B_{s}\right)-m\left(B_{u}\right)}=11 ; \frac{m\left(\Sigma_{c}\right)-m(N)}{m(\Sigma)-m(N)}=6 \tag{1}
\end{equation*}
$$

differ by almost a factor of 2 . The ratio of $m_{s} / m_{l}$ (where $\left.m_{l}=\left(m_{u}+m_{d}\right) / 2\right)$ is known to about $10 \%$ from ratios of squared masses of $K$ and $\pi$ mesons using $\mathrm{SU}(3)$ chiral perturbation theory [1]. Clearly neither ratio is determined well enough this way to provide the accuracy we need, because the relationship between hadron mass and well-defined running quark mass is more complicated than these simple ratios must assume.

Lattice QCD, on the other hand, can give very accurate results for the ratio of two quark masses but only if the same formalism is used for both quarks. This has already been used to give accurate results for $m_{s} / m_{l}$, although neither $m_{s}$ nor $m_{l}$ is very well determined. Here, for the first time, we give an accurate result for $m_{c} / m_{s}$ by using the same formalism for charm, strange and light quarks and this enables us to cascade the accuracy of the heavy quark mass down to the light quarks.

The Lattice QCD calculation. - Lattice QCD gives
direct access to quark masses through the lattice QCD Lagrangian. Tuning of the masses is done by calculating an appropriate hadron mass and adjusting the quark mass until the hadron mass agrees with experiment. Experimental measurements of appropriate hadron masses are extremely accurate in most cases, with errors at the level of tenths or hundredths of a percent. To make maximum use of this precision we need to calculate the hadron mass in lattice QCD with small statistical and systematic errors. In particular it requires the full effect of sea quarks in the hadron to be included. This is now possible in lattice QCD [8]. Fixing the four quark masses $\left(m_{l}\right.$, $m_{s}, m_{c}, m_{b}$ ) from four 'gold-plated' hadrons $\left(\pi, K, \eta_{c}\right.$, $\Upsilon$ ) enables other quantities to be calculated with errors of a few percent and agreement with experiment is obtained [8, 9]. This is an important test that QCD, with only one scale parameter and one mass parameter per quark flavor, describes the full range of hadron physics consistently.

The lattice quark mass is a perfectly well-defined running quark mass. However, it is scheme-dependent and so varies with the discretisation of the Dirac equation used in the lattice calculation. For wider applicability it is more useful to convert the lattice quark mass to a standard continuum scheme such as $\overline{M S}$. This renormalization has been a major source of systematic error in previous determinations of light and strange quark masses. The best existing result for $m_{s}(2 \mathrm{GeV})$, with a $7 \%$ error, uses the direct method of converting the tuned quark mass in the lattice QCD Lagrangian to the $\overline{M S}$ scheme using $\alpha_{s}^{2}$ lattice QCD perturbation theory [10]. The error is dominated by the error in the renormalization and it is the error that we will remove here, by instead determining $m_{c} / m_{s}$ accurately. The Highly Improved Staggered Quark action [11, 12] allows us to use the same discretization of QCD for both charm and strange quarks because it is a fully relativistic 'light quark' action that can also be used for charm quarks. Then the mass renormalisation factor cancels in the quark mass ratio.

We work with eight different ensembles of gluon field configurations provided by the MILC collaboration. These include the effect of $u, d$ and $s$ sea quarks using the improved staggered quark (asqtad) formalism using the fourth root 'trick'. This procedure, although 'ugly', appears to be a valid discretization of QCD 13-16. Tests include studies of the Dirac operator and comparisons to effective field theories. Configurations are available with large spatial volumes $\left(>2.4(\mathrm{fm})^{3}\right)$ at multiple values of the light sea masses (using $m_{u}=m_{d}=m_{l}$ ) and for a wide range of values of the lattice spacing, $a$. We use configurations at five values of $a$ between 0.15 fm and 0.05 fm with parameters as listed in Table $\mathbb{Z}$.

On these configurations we have calculated quark propagators for charm quarks, strange quarks and light quarks (again $m_{u}=m_{d}=m_{l}$ ) using the HISQ action. The numerical speed of HISQ means that we have been able to

| Set $\beta$ | $r_{1} / a$ | $a u_{0} m_{0 l}^{a s q}$ | $a u_{0} m_{0 s}^{a s q}$ | $L / a$ | $T / a$ | $N_{\text {conf }} \times N_{t}$ |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 6.578 | $2.152(5)$ | 0.0097 | 0.0484 | 16 | 48 | $631 \times 2$ |
| 2 | 6.586 | $2.138(4)$ | 0.0194 | 0.0484 | 16 | 48 | $631 \times 2$ |
| 3 | 6.76 | $2.647(3)$ | 0.005 | 0.05 | 24 | 64 | $678 \times 2$ |
| 4 | 6.76 | $2.618(3)$ | 0.01 | 0.05 | 20 | 64 | $595 \times 2$ |
| 5 | 7.09 | $3.699(3)$ | 0.0062 | 0.031 | 28 | 96 | $566 \times 4$ |
| 6 | 7.11 | $3.712(4)$ | 0.0124 | 0.031 | 28 | 96 | $265 \times 4$ |
| 7 | 7.46 | $5.296(7)$ | 0.0036 | 0.018 | 48 | 144 | $201 \times 2$ |
| 8 | 7.81 | $7.115(20)$ | 0.0028 | 0.014 | 64 | 192 | $208 \times 2$ |

TABLE I: Ensembles (sets) of MILC configurations used, with gauge coupling $\beta$, size $L^{3} \times T$ and sea masses ( $\times$ tadpole parameter $\left.u_{0}\right) m_{0 l}^{a s q}$ and $m_{0 s}^{a s q}$. The lattice spacing values in units of $r_{1}$ after 'smoothing' are given in column 3 14. Column 8 gives the number of configurations and time sources per configuration used for calculating correlators.

| Set | $a m_{0 c}$ | $1+\epsilon$ | $a m_{\eta_{c}}$ | $a m_{0 s}$ | $a m_{\eta_{s}}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 0.81 | 0.665 | $2.19381(16)$ | 0.061 | $0.50490(36)$ |
|  | 0.825 | 0.656 | $2.22013(15)$ | 0.066 | $0.52524(36)$ |
|  | 0.85 | 0.641 | $2.26352(15)$ | 0.080 | $0.57828(34)$ |
| 2 | 0.825 | 0.656 | $2.21954(13)$ | 0.066 | $0.52458(35)$ |
| 3 | 0.65 | 0.762 | $1.84578(8)$ | 0.0537 | $0.43118(18)$ |
| 4 | 0.63 | 0.774 | $1.80849(11)$ | 0.0492 | $0.41436(23)$ |
|  | 0.66 | 0.756 | $1.86674(19)$ | 0.0546 | $0.43654(24)$ |
|  | 0.72 | 0.72 | $1.98114(15)$ | 0.05465 | $0.43675(24)$ |
|  | 0.753 | 0.70 | $2.04293(10)$ | 0.06 | $0.45787(23)$ |
|  |  |  |  | 0.063 | $0.46937(24)$ |
| 5 | 0.413 | 0.893 | $1.28057(7)$ | 0.0337 | $0.29413(12)$ |
|  | 0.43 | 0.885 | $1.31691(7)$ | 0.0358 | $0.30332(12)$ |
|  | 0.44 | 0.88 | $1.33816(7)$ | 0.0366 | $0.30675(12)$ |
|  | 0.45 | 0.875 | $1.35934(7)$ | 0.0382 | $0.31362(14)$ |
| 6 | 0.427 | 0.885 | $1.30731(10)$ | 0.03635 | $0.30513(20)$ |
| 7 | 0.273 | 0.951 | $0.89932(12)$ | 0.0228 | $0.20621(19)$ |
|  | 0.28 | 0.949 | $0.91551(9)$ | 0.024 | $0.21196(13)$ |
| 8 | 0.195 | 0.975 | $0.67119(6)$ | 0.0165 | $0.15484(14)$ |
|  |  |  |  | 0.018 | $0.16209(17)$ |

TABLE II: Results for the masses in lattice units of the goldstone pseudoscalars made from valence HISQ charm or strange quarks on the different MILC ensembles enumerated in Table Columns 2 and 3 give the corresponding bare charm quark mass, and Naik coefficient respectively. Column 6 gives the bare strange quark mass ( $\epsilon=0$ in that case).
use several nearby quark masses for charm and strange to allow accurate interpolation to the correct values. Table II gives masses for the goldstone pseudoscalar mesons made from either a charm quark-antiquark pair or a strange one (the $\eta_{c}$ and the $\eta_{s}$ ), which are used for tuning. In the charm case, as well as the quark mass, we list the coefficient of the 'Naik' term in the HISQ action that corrects for discretisation errors through $\left(a m_{0 c}\right)^{4}$. The quark propagators are generated from random wall sources and the goldstone mesons have good signal/noise properties so the meson masses can be determined to high precision using a standard multi-exponential fit [17].

The meson masses can be converted to physical units with a determination of the lattice spacing. On an en-


FIG. 1: Grey points show the raw data for every ratio of $m_{c} / m_{s}$ on each ensemble (Table II); these ratios are fit to eq. 4 The dashed line and associated grey error band (and red point at $a=0$ ) show our extrapolation of the resulting tuned $m_{c} / m_{s}$ to the continuum limit. Blue points with error bars are from a simple interpolation, separately for each ensemble, to the correct $m_{c} / m_{s}$, and are shown for illustration.
semble by ensemble basis this is taken from a parameter in the heavy quark potential called $r_{1}$. Values for $r_{1} / a$ determined by the MILC collaboration [14] are given in Table They have errors of $0.3-0.5 \%$. The physical value for $r_{1}$ must then be obtained by comparing to experimentally known quantities and we use the value $0.3133(23)$ fm obtained from a set of four such quantities, tested for consistency in the continuum limit [18, 19].

Using the information about meson masses that we have on each ensemble we can interpolate to the correct ratio for $a m_{0 c}$ and $a m_{0 s}$ using appropriate continuum values for the masses of the $\eta_{c}$ and $\eta_{s}$. We correct the experimental value of $m_{\eta_{c}}$ of 2.9803 GeV to $m_{\eta_{c}, \text { phys }}=2.9852(34) \mathrm{GeV}$. This allows for electromagnetic effects $(2.4 \mathrm{MeV}) 18$ and $\eta_{c}$ annihilation to gluons $(2.5 \mathrm{MeV})[11$, both of which are missing from our calculation, so increasing the $\eta_{c}$ mass. We take a $50 \%$ error on each of these corrections and also increase the experimental error to 3 MeV to allow for the spread of results from different $\eta_{c}$ production mechanisms [1]. Since the total shift is only around $0.2 \%$ of the $\eta_{c}$ mass it has a negligible effect as can be seen from our error budget below.

The $\eta_{s}$ is not a physical particle in the real world because of mixing with other flavor neutral combinations to make the $\eta$ and $\eta^{\prime}$. However, in lattice QCD, the particle calculated (as here) from only 'connected' quark propagtors does not mix and is a well-defined meson. Its mass must be determined by relating its properties to those of mesons such as the $\pi$ and $K$ that do appear in experiment. From an analysis of the lattice spacing and $m_{l}$-dependence of the $\pi, K$, and $\eta_{s}$ masses we conclude that the value of the $\eta_{s}$ mass in the continuum and physical $m_{l}$ limits is $0.6858(40) \mathrm{GeV}$ [18].

The connection between the $\overline{M S}$ mass at a scale $\mu$ and
the lattice bare quark mass is given by [10, 20]:

$$
\begin{gather*}
\bar{m}(\mu)=\frac{a m_{0}}{a} Z_{m}\left(\mu a, m_{0} a\right)  \tag{2}\\
Z_{m}=1+\alpha_{s}\left(-\frac{2}{\pi} \log (\mu a)+C+b\left(a m_{0}\right)^{2}+\ldots\right)+\ldots
\end{gather*}
$$

From these two equations it is clear that

$$
\begin{equation*}
\frac{\bar{m}_{c}(\mu)}{\bar{m}_{s}(\mu)}=\left.\frac{a m_{0 c}}{a m_{0 s}}\right|_{\mathrm{phys}} \tag{3}
\end{equation*}
$$

where phys denotes extrapolation to the continuum limit and physical sea quark mass limit.

On each ensemble the ratios we have for $a m_{0 c} / a m_{0 s}$ then differ from the physical value because of three effects: mistuning from the correct physical meson mass; finite $a$ effects that need to be extrapolated away and effects because the sea light quark masses are not correct. We incorporate these into our fitting function:

$$
\begin{align*}
& \left.\frac{m_{0 c}}{m_{0 s}}\right|_{\text {lat }}=\left.\frac{m_{0 c}}{m_{0 s}}\right|_{\text {phys }} \times\left(1+d_{\text {sea }} \frac{\delta m_{\mathrm{tot}}^{\mathrm{sea}}}{m_{s}}\right)  \tag{4}\\
& \times\left(1+\sum_{i, j, k, l} c_{i j k l} \delta_{c}^{i} \delta_{s}^{j}\left(\frac{a m_{\eta_{c}}}{2}\right)^{2 k}\left(a m_{\eta_{s}}\right)^{2 l}\right) \\
& \delta_{c}=\frac{m_{\eta_{c}, M C}-m_{\eta_{c}, \text { phys }}}{m_{\eta_{c}, \text { phys }}} ; \delta_{s}=\frac{m_{\eta_{s}, M C}^{2}-m_{\eta_{s}, \text { phys }}^{2}}{m_{\eta_{s}, \text { phys }}^{2}} \tag{5}
\end{align*}
$$

are the measures of mistuning, where $M C$ denotes lattice values converted to physical units. The last bracket fits the finite lattice spacing effects as a power series in even powers of $a$. These can either have a scale set by $m_{c}$ (for which we use $a m_{\eta_{c}} / 2$ ) or by $\Lambda_{Q C D}$ (for which we use $\left.a m_{\eta_{s}}\right) . i, j, k, l$ all start from zero and are varied in the ranges: $i, j \leq 3, k \leq 6, l \leq 2$ with $i+j+k+l \leq 6$. Doubling any of the upper limits has negligible effect on the final result. The prior on $c_{i j k l}$ is set to $0(1)$. $\delta m_{\text {tot }}^{\text {sea }}$ is the total difference between the sea-quark masses used in the simulation and the correct value for $2 m_{l}+m_{s}$ [18]. This has a tiny effect and we simply use a linear term (adding higher orders has negligible effect). The prior for $d_{\text {sea }}$ is $0.0(1)$. Figure 1 shows the results of the fit, giving $m_{c} / m_{s}$ in the continuum limit as $11.85(16)\left(\chi^{2} /\right.$ dof $=$ 0.42 ). The error budget is given in Table III.
$m_{s} / m_{l}$ is known to $1 \%$ from lattice QCD as a byproduct of standard chiral extrapolations of $m_{\pi}^{2}$ and $m_{K}^{2}$ to the physical point [21]. MILC quote 27.2(3) using asqtad quarks [14. Our HISQ analysis in [12] gave a result in agreement at 27.8(3), using a Bayesian fit to a function including terms from chiral perturbation theory up to third order in $m_{l}$ and allowing for discretisation errors up to and including $a^{4}$ and for mixed terms (i.e $m_{l}$-dependent discretisation errors). A full error budget is given in Table III, the data are given in [18].

|  | $m_{c} / m_{s} m_{s} / m_{l}$ |  |
| :--- | :--- | :--- |
| overall $r_{1}$ uncertainty | $0.4 \%$ | $0.1 \%$ |
| $r_{1} / a$ uncertainties | 0.2 | - |
| continuum $M_{\eta_{c}}$ | 0.2 | - |
| continuum $M_{\eta_{s}}$ | 1.1 | - |
| Finite volume | - | 0.3 |
| $a^{2}$ extrapolation, $m_{q}$ interpolns | 0.4 | 0.8 |
| sea-quark mass extrapolation | 0.0 | 0.2 |
| statistical errors | 0.3 | 0.4 |
| Total | $1.3 \%$ | $1.0 \%$ |

TABLE III: Error budgets for $m_{c} / m_{s}$ and $m_{s} / m_{l}$.

Conclusions. - Our $m_{c} / m_{s}$ can be used with any value for $m_{c}$ to give $m_{s}$. The best existing result [4] (converted from $n_{f}=4$ to 3 ) is $\bar{m}_{c}^{(3)}(2.0 \mathrm{GeV})=1.095(11) \mathrm{GeV}$ or $\bar{m}_{c}^{(3)}(3.0 \mathrm{GeV})=0.990(10) \mathrm{GeV}$. Dividing by $11.85(16)$ gives $\bar{m}_{s}^{(3)}(2.0 \mathrm{GeV})=92.4(1.5) \mathrm{MeV}$ and $\bar{m}_{s}^{(3)}(3.0 \mathrm{GeV})$ $=83.5(1.4) \mathrm{MeV}$.


FIG. 2: Our results for the 4 lightest quark masses compared to the current PDG evaluations (shaded bands) [1]. Each mass is quoted in the $\overline{M S}$ scheme at its conventional scale: 2 GeV for $u, d, s\left(n_{f}=3\right) ; m_{c}$ for $c\left(n_{f}=4\right)$.

Using the MILC values for $m_{s} / m_{l}$ and $m_{u} / m_{d}$ (0.42(4) [14]) we can then obtain: $\bar{m}_{l}^{(3)}(2.0 \mathrm{GeV})$ $=3.40(7) \mathrm{MeV}$ and $\bar{m}_{l}^{(3)}(3.0 \mathrm{GeV})=3.07(6) \mathrm{MeV}$; $\bar{m}_{u}^{(3)}(2.0 \mathrm{GeV})=2.01(14) \mathrm{MeV}$ and $\bar{m}_{d}^{(3)}(2.0 \mathrm{GeV})=$ 4.79 (16) MeV . The values for all four quark masses are plotted in Figure 2 in comparison to the current evaluations from the Particle Data Tables [1].

Thus our high accuracy on $m_{c} / m_{s}$ allows us to leverage $2 \%$ accurate values for $m_{s}$ and $m_{l}$ that are completely nonperturbative in lattice QCD , for the first time. Our $m_{s}$ mass is higher, by around $1 \sigma$, than our previous value of $\bar{m}_{s}(2 \mathrm{GeV})=87(6) \mathrm{MeV}$ which used 2-loop lattice QCD perturbation theory [10]. Then the error was dominated by unknown $\alpha_{s}^{3}$ terms. Our new result, which does not have this limitation, has an error almost five times smaller. Our new error is almost an order of magnitude smaller than other lattice QCD results from full

QCD [22, 23]. These use direct methods of converting the lattice mass to the $\overline{M S}$ mass, and have $10 \%$ errors.

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# High-Precision $c$ and $b$ Masses, and QCD Coupling from Current-Current Correlators in Lattice and Continuum QCD 

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#### Abstract

We extend our earlier lattice-QCD analysis of heavy-quark correlators to smaller lattice spacings and larger masses to obtain new values for the $c$ mass and QCD coupling, and, for the first time, values for the $b$ mass: $m_{c}\left(3 \mathrm{GeV}, n_{f}=4\right)=0.986(6) \mathrm{GeV}, \alpha_{\overline{\mathrm{MS}}}\left(M_{Z}, n_{f}=5\right)=0.1183(7)$, and $m_{b}\left(10 \mathrm{GeV}, n_{f}=5\right)=3.617(25) \mathrm{GeV}$. These are among the most accurate determinations by any method. We check our results using a nonperturbative determination of the mass ratio $m_{b}\left(\mu, n_{f}\right) / m_{c}\left(\mu, n_{f}\right)$; the two methods agree to within our $1 \%$ errors and taken together imply $m_{b} / m_{c}=4.51(4)$. We also update our previous analysis of $\alpha_{\overline{M S}}$ from Wilson loops to account for revised values for $r_{1}$ and $r_{1} / a$, finding a new value $\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}, n_{f}=5\right)=0.1184(6)$; and we update our recent values for light-quark masses from the ratio $m_{c} / m_{s}$. Finally, in the Appendix, we derive a procedure for simplifying and accelerating complicated least-squares fits.


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## I. INTRODUCTION

Precise values for the QCD coupling $\alpha_{\overline{\mathrm{MS}}}$ and the quark masses are important for high-precision tests of the Standard Model of particle physics. In a recent paper we showed how to use realistic lattice QCD simulations to extract both the coupling and the charm quark's mass $m_{c}$ from zero-momentum moments of correlators built from the $c$ quark's (UV cutoff-independent) pseudoscalar density operator $m_{c} \bar{\psi}_{c} \gamma_{5} \psi_{c}$ [1]. In this paper we refine our previous analysis and extend it to include other quark masses, up to and including the $b$-quark mass. As a result our coupling constant and mass determinations from these correlators are among the most accurate by any method.

Low moments of heavy-quark correlators are perturbative and several are now known through $\mathcal{O}\left(\alpha_{s}^{3}\right)$ in perturbation theory (that is, four-loop order) [2-6]. Moments of correlators built from the electromagnetic currents can be estimated nonperturbatively, using dispersion relations, from experimental data for the electron-positron annihilation cross section, $\sigma\left(e^{+} e^{-} \rightarrow \gamma^{*} \rightarrow X\right)$. Accurate values for both the $c$ and $b$ masses can be obtained by comparing these perturbative and nonperturbative determinations of the moments (for a recent discussion see [7]).

In our earlier paper we showed that heavy-quark correlator moments are easily and accurately computed nonperturbatively using lattice QCD simulations, in place of experimental data, provided: 1) the electromagnetic

[^296]current is replaced by the pseudoscalar density multiplied by the bare quark mass; 2) the discretization of the quark action has a partially conserved axial vector current (PCAC); and 3) the discretization remains accurate when applied to heavy quarks. In our simulations we use the HISQ discretization of the quark action, which is a highly corrected version of the standard staggeredquark action [8]. It has a chiral symmetry (PCAC) and has been used in a wide variety of accurate simulations involving $c$ quarks [8-12].

Here we show that the HISQ action can be pushed to still higher masses - indeed, very close to the $b$ mass on new lattices, from the MILC collaboration [13], with the smallest lattice spacings available today ( 0.044 fm ). Currently most high-precision lattice work on $b$ physics relies upon nonrelativistic effective field theories, like NRQCD 10, 12, 14, 15]. In this paper we show how to obtain accurate $b$ physics using the fully relativistic HISQ action on these new lattices.

In what follows, we first review how the QCD coupling and quark masses are extracted from heavy-quark correlators, in Section II. Then in Section III we describe our lattice QCD simulations and discuss in detail the chief systematic errors in our simulation results. In Section IV we describe our fitting procedure and the results of our analysis of the heavy-quark correlators. We check our calculation using a different, nonperturbative method to determine $m_{b} / m_{c}$ in Section V. We then, in Section VI, update our previous calculation of the QCD coupling from Wilson loops to compare with our new result from the correlators. We summarize our findings in Section VII and compare our results with work by others. There we also update our recent calculations of the light-quark masses from the $c$ mass. In the Appendix we present a powerful simplification for complicated least-
squares fits that can greatly reduce the computing required for fits. We use this technique in dealing with finite- $a$ errors in our analysis.

## II. HEAVY-QUARK CORRELATOR MOMENTS

Following our earlier paper [1], we focus on correlators formed from the pseudoscalar density of a heavy quark, $j_{5}=\bar{\psi}_{h} \gamma_{5} \psi_{h}:$

$$
\begin{equation*}
G(t)=a^{6} \sum_{\mathbf{x}}\left(a m_{0 h}\right)^{2}\langle 0| j_{5}(\mathbf{x}, t) j_{5}(0,0)|0\rangle \tag{1}
\end{equation*}
$$

where $m_{0 h}$ is the heavy quark's bare mass (from the lattice QCD lagrangian), $t$ is euclidean and periodic with period $T$, and the sum over spatial positions $\mathbf{x}$ sets the total three momentum to zero. In our earlier paper we examined only $c$ quarks; here we will consider a range of masses between the $c$ and $b$ masses. While we have written this formula for use with the lattice regulator, it is important to note that the correlator is UV-finite because we include the factors of $a m_{0 h}$. Consequently lattice and continuum $G(t)$ s are equal when $t \neq 0$ up to $\mathcal{O}\left(\left(a m_{h}\right)^{m}\right)$ corrections, which vanish in the continuum limit.

The moments of $G(t)$ are particularly simple to analyze:

$$
\begin{equation*}
G_{n} \equiv \sum_{t}(t / a)^{n} G(t) \tag{2}
\end{equation*}
$$

where, on our periodic lattice,

$$
\begin{equation*}
t / a \in\{0,1,2 \ldots T / 2 a-1,0,-T / 2 a+1 \ldots-2,-1\} \tag{3}
\end{equation*}
$$

Low moments emphasize small $t$ s and so are perturbative; and moments with $n \geq 4$ are UV-cutoff independent. Therefore

$$
\begin{equation*}
G_{n}=\frac{g_{n}\left(\alpha_{\overline{\mathrm{MS}}}(\mu), \mu / m_{h}\right)}{\left(a m_{h}(\mu)\right)^{n-4}}+\mathcal{O}\left(\left(a m_{h}\right)^{m}\right) \tag{4}
\end{equation*}
$$

for small $n \geq 4$, where $m_{h}(\mu)$ is the heavy quark's $\overline{\mathrm{MS}}$ mass at scale $\mu$, and the dimensionless factor $g_{n}$ can be computed using continuum perturbation theory.

Again following our previous paper, we introduce reduced moments to suppress both lattice artifacts and tuning errors in the heavy quark's mass [16]:

$$
R_{n} \equiv \begin{cases}G_{4} / G_{4}^{(0)} & \text { for } n=4  \tag{5}\\ \frac{a m_{\eta_{h}}}{2 a m_{0 h}}\left(G_{n} / G_{n}^{(0)}\right)^{1 /(n-4)} & \text { for } n \geq 6\end{cases}
$$

where $G_{n}^{(0)}$ is the moment in lowest-order, weak-coupling perturbation theory, using the lattice regulator, and $m_{\eta_{h}}$ is the (nonperturbative) mass of the pseudo-Goldstone $h \bar{h}$ boson. The reduced moments can again be written in terms of continuum quantities:

$$
R_{n} \equiv \begin{cases}r_{4}\left(\alpha_{\overline{\mathrm{MS}}}, \mu / m_{h}\right) & \text { for } n=4  \tag{6}\\ z\left(\mu / m_{h}, m_{\eta_{h}}\right) r_{n}\left(\alpha_{\overline{\mathrm{MS}}}, \mu / m_{h}\right) & \text { for } n \geq 6\end{cases}
$$

up to $\mathcal{O}\left(\left(a m_{h}\right)^{m} \alpha_{s}\right)$ corrections, where

$$
\begin{equation*}
z\left(\mu / m_{h}, m_{\eta_{h}}\right) \equiv \frac{m_{\eta_{h}}}{2 m_{h}(\mu)}, \tag{7}
\end{equation*}
$$

and $r_{n}$ is obtained from $g_{n}$ (Eq. (4)) and its value, $g_{n}^{(0)}$, in lowest-order continuum perturbation theory:

$$
r_{n}= \begin{cases}g_{4} / g_{4}^{(0)} & \text { for } n=4  \tag{8}\\ \left(g_{n} / g_{n}^{(0)}\right)^{1 /(n-4)} & \text { for } n \geq 6\end{cases}
$$

Our strategy for extracting quark masses and the QCD coupling relies upon lattice simulations to determine nonperturbative values for the $R_{n}$, using simulation results for $a m_{\eta_{h}} / a m_{0 h}$. We then compare this simulation "data" to the continuum perturbation theory formulas (Eq. (6)). That is, we find values for $\alpha_{\overline{\mathrm{MS}}}(\mu)$ and $z\left(\mu / m_{h}, m_{\eta_{h}}\right)$ that make lattice and continuum results agree for small $n \geq 4$. The function $z\left(\mu / m_{h}, m_{\eta_{h}}\right)$ can then be combined with experimental results for $m_{\eta_{c}}$ and $m_{\eta_{b}}$ to obtain masses for the $c$ and $b$ quarks:

$$
\begin{equation*}
m_{c}(\mu)=\frac{m_{\eta_{c}}^{\exp }}{2 z\left(\mu / m_{c}, m_{\eta_{c}}^{\exp }\right)} \quad m_{b}(\mu)=\frac{m_{\eta_{b}}^{\exp }}{2 z\left(\mu / m_{b}, m_{\eta_{b}}^{\exp }\right)} \tag{9}
\end{equation*}
$$

Parameter $\mu$ sets the scale for $\alpha_{\overline{\mathrm{MS}}}$ in the perturbative expansions of the $r_{n}$. An obvious choice for this parameter is $\mu=m_{h}$ since the quark mass, together with $n$, sets the momentum scale in our correlators. As noted in our previous paper, however, perturbation theory is somewhat more convergent if we use larger $\mu \mathrm{s}$ in the $c$ quark case. Consequently here we take $\mu / m_{h}=3$, which is approximately what we did in our previous paper.

The mass and coupling determinations were done separately in our previous paper. Here we extract them simultaneously, to guarantee consistency between results. Also in our previous paper we considered only heavyquark masses near the $c$ mass. Here we explore a variety of masses ranging from just below the $c$ mass to just below the $b$ mass. This allows us to obtain a value for $b$-quark's mass.

## III. LATTICE QCD SIMULATIONS

## A. Simulation Results

The gluon-configuration sets we use were created by the MILC collaboration. The relevant simulation parameters are listed in Table I

Given a lattice spacing, the QCD action is specified completely by the values of the bare coupling constant and the bare quark masses. In our analyses we set the $u$ and $d$ quark masses equal; this approximation results in negligible errors ( $\ll 1 \%$ ) for the quantities studied in this paper. It is too costly to simulate QCD at the correct value for the $u / d$ mass; we typically use masses that are $2-5$ times too large and extrapolate to values that give

TABLE I: Parameter sets used to generate the gluon configurations analyzed in this paper. The lattice spacing is specified in terms of the static-quark potential parameter $r_{1}=0.3133(23) \mathrm{fm}$; values for $r_{1} / a$ are from 13]. The bare quark masses are for the ASQTAD formalism and $u_{0}$ is the fourth root of the plaquette. The spatial $(L)$ and temporal $(T)$ lengths of the lattices are also listed, as are the number of gluon configurations ( $N_{\mathrm{cf}}$ ) and the number of time sources ( $N_{\mathrm{ts}}$ ) per configuration used in each case. Sets with similar lattice spacings are grouped.

| Set | $r_{1} / a$ | $a u_{0} m_{0 u / d}$ | $a u_{0} m_{0 s}$ | $u_{0}$ | $L / a$ | $T / a$ | $N_{\text {cf }} \times N_{\text {ts }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | $2.152(5)$ | 0.0097 | 0.0484 | 0.860 | 16 | 48 | $631 \times 2$ |
| 2 | $2.138(4)$ | 0.0194 | 0.0484 | 0.861 | 16 | 48 | $631 \times 2$ |
| 3 | $2.647(3)$ | 0.005 | 0.05 | 0.868 | 24 | 64 | $678 \times 2$ |
| 4 | $2.618(3)$ | 0.01 | 0.05 | 0.868 | 20 | 64 | $595 \times 2$ |
| 5 | $2.618(3)$ | 0.01 | 0.05 | 0.868 | 28 | 64 | $269 \times 2$ |
| 6 | $3.699(3)$ | 0.0062 | 0.031 | 0.878 | 28 | 96 | $566 \times 4$ |
| 7 | $3.712(4)$ | 0.0124 | 0.031 | 0.879 | 28 | 96 | $265 \times 4$ |
| 8 | $5.296(7)$ | 0.0036 | 0.018 | 0.888 | 48 | 144 | $201 \times 2$ |
| 9 | $7.115(20)$ | 0.0028 | 0.014 | 0.895 | 64 | 192 | $208 \times 2$ |

the correct mass for the $\pi^{0}$-meson. We tune the strange quark mass to give the correct mass for the (fictitious) $\eta_{s}$ meson [10]. The $c$ and $b$ masses are tuned to give correct masses for the $\eta_{c}$ and $\eta_{b}$ mesons, respectively.

It is convenient in QCD simulations to specify a value for the bare coupling constant and then extract the value of the lattice spacing from the simulation. We set the lattice spacing using MILC results for $r_{1} / a$, computed from the heavy-quark potential, and [10]

$$
\begin{equation*}
r_{1}=0.3133(23) \mathrm{fm} \tag{10}
\end{equation*}
$$

The MILC configurations include vacuum polarization contributions from only the lightest three quark flavors, using the ASQTAD discretization. Vacuum polarization effects from the heavier $c$ and $b$ quarks are easily incorporated into our final results for quark masses and the QCD coupling using perturbation theory.

We computed heavy-quark correlators (Eq. (11) using the HISQ discretization [8] for a variety of bare heavyquark masses $a m_{0 h}$ on the MILC gluon configurations. Our results for the reduced moments $R_{n}$ with $n=4-18$ are given in Table II.

In Table II, we also give masses $a m_{\eta_{h}}$ from the simulations for the pseudo-Goldstone meson made from two heavy quarks. These were computed using singleexponential fits to $G(t)$ for the middle $30 \%$ of $t$ s on the lattice for all configurations except the two smallest lattice spacings where we used only $8 \%$ of the $t$. We have less statistics for the two finest lattice spacings and consequently the fits did not work as well for these. We increased the statistical errors on our results for $a m_{\eta_{h}}$ by factors of 1.4 and 2 for the next-to-finest and finest lattice spacings (sets 8 and 9 ), respectively, to account for this. The statistical errors here are very small and have only a small impact on our final results. We also verified our results with multi-exponential fits in every case.

## B. Systematic Errors

As discussed above, our goal is to find values for $\alpha_{\overline{\mathrm{MS}}}(\mu)$ and $z\left(\mu / m_{h}, m_{\eta_{h}}\right)$ (Eq. (77)) that make the theoretical results from perturbative QCD agree, to within statistical and systematic errors, with Monte Carlo simulation "data" for the reduced moments. We simultaneously analyze results for all of our lattice spacings and most of our masses, and for moments with $4 \leq n \leq 10$. We focus on these particular moments for our final results since their perturbation theory is known to third order.

Systematic errors are larger here than statistical errors, which contribute less than $0.3 \%$. We discuss the most important sources of systematic error in this section.

## 1. $m_{h}$ Extrapolations

We need the $m_{\eta_{h}}$ dependence of the mass-ratio function $z\left(\mu / m_{h}=3, m_{\eta_{h}}\right)$ in order to extract $c$ and $b$ masses from our simulation (using Eq. (9)). We parameterize this dependence as follows:

$$
\begin{equation*}
z\left(\mu / m_{h}, m_{\eta_{h}}\right)=\sum_{j=0}^{N_{z}} z_{j}\left(\mu / m_{h}\right)\left(\frac{2 \Lambda}{m_{\eta_{h}}}\right)^{j} \tag{11}
\end{equation*}
$$

where the $z_{j}$ s are determined in our fit. This is an expansion in the QCD scale, which we take to be

$$
\begin{equation*}
\Lambda=0.5 \mathrm{GeV} \tag{12}
\end{equation*}
$$

divided by $m_{\eta_{h}} / 2$, which we use as a proxy for the quark mass. The expansion is adequate for the range of quark masses used in our analysis, where $\left(2 \Lambda / m_{\eta_{h}}\right)^{2}$ ranges approximately between $1 / m_{\eta_{b}}^{2}=0.01$ and $\left(1 / m_{\eta_{c}}\right)^{2}=0.1$; the singular point $m_{h}=0$ is infinitely far away in this parameterization. In our fits we keep terms only through order $N_{z}=4$, but, as we discuss later, our results are unchanged by additional terms. On dimensional grounds, we assume a priori that the coefficients are

$$
\begin{equation*}
z_{j}(3)=0 \pm 1 \tag{13}
\end{equation*}
$$

## 2. Finite-Lattice Spacing Errors

Discretization errors are of order $\left(a m_{h}\right)^{2 i} \alpha_{s}$ for $i \geq 1$. We model these by

$$
\begin{equation*}
R_{n}^{\text {latt }}=R_{n}\left(\mu, m_{\eta_{h}}, a, N_{a m}\right) \tag{14}
\end{equation*}
$$

where: fit function $R_{n}\left(\mu, m_{\eta_{h}}, a, N_{a m}\right)$ has the double expansion

$$
\begin{align*}
& R_{n}\left(\mu, m_{\eta_{h}}, a, N_{a m}\right) \equiv R_{n}^{\mathrm{cont}} /  \tag{15}\\
& \qquad\left(1+\sum_{i=1}^{N_{a m}} \sum_{j=0}^{N_{z}} c_{i j}^{(n)}\left(\frac{a m_{\eta_{h}}}{2}\right)^{2 i}\left(\frac{2 \Lambda}{m_{\eta_{h}}}\right)^{j}\right)
\end{align*}
$$

TABLE II: Results for the reduced moments $R_{n}$ and pseudoscalar-meson mass $a m_{\eta_{h}}$ obtained from ( $n_{f}=3$ ) simulations using different bare heavy-quark (HISQ) masses $a m_{0 h}$ and gluon configuration sets (see Table I). The errors listed here are statistical errors from the Monte Carlo simulation. Results where $a m_{\eta_{h}}>1.95$ are omitted from our final analysis, as are $R_{n} s$ with $n>10$.

| Set | $a m_{0 h}$ | $a m_{\eta}$ | $R_{4}$ | $R_{6}$ | $R_{8}$ | $R_{10}$ | $R_{12}$ | $R_{14}$ | $R_{16}$ | $R_{18}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0.660 | 1.9202(1) | 1.2132(3) | 1.5364(3) | 1.4151(2) | 1.3476(1) | 1.3001(1) | 1.2649(1) | 1.2378(1) | 1.2164(1) |
|  | 0.810 | 2.1938(1) | 1.1643(2) | 1.4427(2) | 1.3619(1) | 1.3148(1) | 1.2780(1) | 1.2481(1) | 1.2238(1) | 1.2039(1) |
|  | 0.825 | 2.2202(1) | 1.1604(2) | 1.4339(2) | 1.3563(1) | 1.3111(1) | 1.2754(1) | 1.2462(1) | 1.2222(1) | 1.2025(1) |
| 2 | 0.825 | 2.2196(1) | 1.1591(2) | 1.4327(2) | 1.3556(1) | 1.3106(1) | 1.2751(1) | 1.2459(1) | 1.2221(1) | 1.2024(1) |
| 3 | 0.650 | 1.8458(1) | 1.1809(2) | $1.4805(2)$ | 1.3755(1) | 1.3160(1) | 1.2740(1) | 1.2429(1) | 1.2190(1) | 1.2000(1) |
| 4 | 0.440 | 1.4241(1) | 1.2752(4) | 1.6144(4) | 1.4397(2) | 1.3561(2) | 1.3041(1) | 1.2678(1) | 1.2408(1) | 1.2200(1) |
|  | 0.630 | 1.8085(1) | 1.1881(3) | 1.4935(2) | 1.3826(1) | 1.3205(1) | 1.2773(1) | 1.2456(1) | 1.2214(1) | 1.2021(1) |
|  | 0.660 | 1.8667(1) | 1.1782(2) | 1.4764(2) | 1.3738(1) | 1.3152(1) | 1.2736(1) | 1.2426(1) | 1.2187(1) | 1.1997(1) |
|  | 0.720 | 1.9811(1) | 1.1605(2) | 1.4435(2) | 1.3559(1) | 1.3044(1) | 1.2662(1) | 1.2367(1) | 1.2136(1) | 1.1950(1) |
|  | 0.850 | 2.2194(1) | 1.1301(2) | 1.3763(1) | 1.3145(1) | 1.2774(1) | 1.2473(1) | 1.2221(1) | 1.2012(1) | 1.1839(1) |
| 5 | 0.630 | 1.8086(1) | 1.1882(1) | 1.4936(1) | 1.3826(1) | 1.3205(1) | 1.2774(1) | 1.2457(1) | 1.2214(0) | 1.2022(0) |
| 6 | 0.300 | 1.0314(1) | 1.2930(3) | 1.6061(3) | 1.4249(2) | 1.3444(1) | 1.2953(1) | 1.2610(1) | 1.2353(1) | 1.2153(1) |
|  | 0.413 | 1.2806(1) | 1.2224(2) | 1.5216(2) | 1.3796(1) | 1.3115(1) | 1.2689(1) | 1.2390(1) | 1.2164(1) | 1.1985(1) |
|  | 0.430 | 1.3169(1) | 1.2145(2) | 1.5113(2) | 1.3743(1) | 1.3076(1) | 1.2658(1) | 1.2363(1) | 1.2141(1) | 1.1964(1) |
|  | 0.440 | 1.3382(1) | 1.2100(2) | 1.5054(2) | 1.3712(1) | 1.3054(1) | 1.2640(1) | 1.2348(1) | 1.2127(1) | 1.1952(1) |
|  | 0.450 | 1.3593(1) | 1.2057(2) | 1.4996(2) | 1.3683(1) | 1.3033(1) | 1.2623(1) | 1.2333(1) | 1.2114(1) | 1.1941(1) |
|  | 0.700 | 1.8654(1) | 1.1301(1) | 1.3782(1) | 1.3053(1) | 1.2616(1) | 1.2294(1) | 1.2048(0) | 1.1857(0) | $1.1705(0)$ |
|  | 0.850 | 2.1498(1) | 1.1026(1) | 1.3163(1) | 1.2671(1) | 1.2366(0) | $1.2114(0)$ | 1.1903(0) | 1.1729(0) | 1.1584(0) |
| 7 | 0.427 | 1.3074(1) | 1.2131(3) | 1.5091(3) | 1.3729(2) | 1.3066(1) | 1.2651(1) | 1.2358(1) | 1.2137(1) | 1.1961(1) |
| 8 | 0.273 | 0.8993(3) | 1.2454(8) | 1.5234(9) | 1.3739(7) | 1.3069(6) | $1.2657(6)$ | 1.2366(6) | 1.2145(6) | 1.1969(5) |
|  | 0.280 | 0.9154(2) | 1.2403(5) | 1.5175(5) | 1.3706(3) | 1.3045 (3) | 1.2638(2) | 1.2350(2) | 1.2132(2) | 1.1958(2) |
|  | 0.564 | 1.5254(1) | 1.1324(2) | 1.3674(2) | $1.2857(2)$ | 1.2405(1) | 1.2102(1) | 1.1885(1) | 1.1719(1) | 1.1587(1) |
|  | 0.705 | 1.8084(1) | 1.1043(2) | 1.3156(2) | 1.2574(1) | 1.2217(1) | 1.1952(1) | 1.1750(1) | 1.1593(1) | 1.1467(1) |
|  | 0.760 | 1.9157(1) | 1.0955(2) | 1.2965(2) | 1.2460(1) | 1.2142(1) | 1.1895(1) | 1.1701(1) | 1.1547(1) | 1.1423(1) |
|  | 0.850 | 2.0875(1) | 1.0831(2) | 1.2666(1) | 1.2266(1) | 1.2010(1) | 1.1799(1) | 1.1621(1) | 1.1474(1) | 1.1353(1) |
| 9 | 0.195 | 0.6710(2) | 1.2583(5) | 1.5243(5) | 1.3733(4) | 1.3066(3) | 1.2655(3) | 1.2364(2) | 1.2144(2) | 1.1968(2) |
|  | 0.400 | 1.1325(2) | 1.1532(3) | 1.3800(3) | 1.2838(2) | 1.2370 (2) | 1.2077(2) | 1.1869(2) | 1.1710 (2) | 1.1583(2) |
|  | 0.500 | 1.3446(2) | 1.1267(2) | 1.3410(2) | 1.2616(1) | 1.2198(1) | 1.1927(1) | 1.1734(1) | 1.1588(1) | 1.1471(1) |
|  | 0.700 | 1.7518(1) | 1.0900(1) | 1.2765(1) | 1.2261(1) | 1.1949(1) | 1.1718(1) | 1.1542(1) | 1.1407(1) | 1.1299(1) |
|  | 0.850 | 2.0428(1) | 1.0712(1) | 1.2327(1) | 1.1983(1) | 1.1760(1) | 1.1574(1) | 1.1418(1) | 1.1290(1) | 1.1185(1) |

the $c_{i j}^{(n)} \mathrm{s}$ are determined in our fit, $R_{n}^{\text {cont }}$ is given by Eq. (6),

$$
\begin{equation*}
i+j \leq \max \left(N_{a m}, N_{z}\right) \tag{16}
\end{equation*}
$$

and again we use $m_{\eta_{h}} / 2$ in place of the quark mass. This expansion allows for finite- $a$ corrections involving $\left(a m_{\eta_{h}} / 2\right)^{2},(a \Lambda)^{2}$, and cross terms, with $m_{\eta_{h}}$-dependent coefficients. We assume a priori that

$$
\begin{equation*}
c_{i j}^{(n)}=0 \pm 2 / n \tag{17}
\end{equation*}
$$

which implies smaller $a$ dependence for larger $n \mathrm{~s}$. This is expected (and obvious in our simulation data) since the reduced moments become more infrared as $n$ increases. The exact functional form of the $n$ dependence has little effect on our results, as we show later.

In our fits we take $N_{z}=4$. While low orders suffice for the $2 \Lambda / m_{\eta_{h}}$ expansion, expansion parameter $a m_{\eta_{h}} / 2$ ranges between 0.3 and 1.1, and higher orders are necessary, especially given our tiny statistical errors. We find that our fit results don't converge well unless $N_{a m}$ is larger than 10-20. Also we have difficulty getting good fits if we include data with $a m_{\eta_{h}}>1.95$ from Table II

The $a m_{\eta_{h}} / 2$ expansion may not converge for these last cases and therefore we exclude such data from our final analysis.

The fit function has many more fit parameters $c_{i j}^{(n)}$ than we have simulation data points when $N_{a m}$ is so large. This does not cause problems in (Bayesian) constrained fits since the parameters' priors (Eq. (17)) are included in the fit as extra data [17]. Each parameter has a prior and therefore we always have more data than parameters.

It is, however, very time consuming to fit a function with so many fit parameters. Although it is not essential for our analysis, there is a trick that greatly accelerates this kind of fit. The idea is to fit a modified moment $\bar{R}_{n}^{\text {latt }}$ in place of $R_{n}^{\text {latt }}$ where

$$
\begin{align*}
& \bar{R}_{n}^{\text {latt }} \equiv R_{n}^{\mathrm{latt}}+  \tag{18}\\
& R_{n}^{\mathrm{latt}} \sum_{i=\bar{N}_{a m}+1}^{N_{a m}} \sum_{j=0}^{N_{z}} c_{i j}^{(n)}\left(\frac{a m_{\eta_{h}}}{2}\right)^{2 i}\left(\frac{2 \Lambda}{m_{\eta_{h}}}\right)^{j} .
\end{align*}
$$

and $\bar{N}_{a m} \ll N_{a m}$. The modified moment is fit with the
much simpler formula (simpler since $\bar{N}_{a m} \ll N_{a m}$ )

$$
\begin{equation*}
\bar{R}_{n}^{\text {latt }}=R_{n}\left(\mu, m_{\eta_{h}}, a, \bar{N}_{a m}\right) \tag{19}
\end{equation*}
$$

where $R_{n}(\ldots)$ is again given by Eq. (15). To evaluate $\bar{R}_{n}^{\text {latt }}$ from Eq. (18), we treat the coefficients $c_{i j}^{(n)}$ with $i>\bar{N}_{a m}$ as new data with means and standard deviations specified by the prior, Eq. (17). Uncertainties coming from the $c_{i j}^{(n)} \mathrm{s}$ are combined in quadrature with the statistical error in $R_{n}^{\text {latt }}$ to obtain a new error estimate for $\bar{R}_{n}^{\text {latt }}$ (but leaving the central value unchanged). In effect we are increasing the error in the reduced moment to account for high-order $\left(a m_{\eta_{h}} / 2\right)^{2 i}$ terms omitted from the fit formula Eq. (19). By choosing $\bar{N}_{a m} \ll N_{a m}$, most of the $a m_{\eta_{h}} / 2$ terms are incorporated into $\bar{R}_{n}^{\text {latt }}$ (Eq. (18)), where they are inexpensive, and relatively few end up in the fit function $\bar{R}_{n}(\ldots)$ (Eq. (15)), where they add parameters to the fit and increase its cost. Note that the new errors introduce correlations between $\bar{R}_{n}^{\text {latt }} \mathrm{S}$ computed with different lattice spacings or quark masses, since the same $c_{i j}^{(n)}$ s are used for all $a$ s and $m_{\eta_{h}} \mathrm{~s}$. These correlations are important and need to be preserved in the fit.

Our procedure, whereby terms are moved out of the fitting function and incorporated into new (correlated) errors in the Monte Carlo fit data, is generally useful. Somewhat remarkably, final fit results are completely (or almost completely) independent of the number of terms that are transferred when fits are linear (or almost linear) in the associated parameters. (The general theorem from which this result follows is proven in the Appendix.) Consequently, in our analysis here, we can take $N_{a m}$ very large-say, $N_{a m}=80$ - and still have very fast fits by keeping $\bar{N}_{a m}$ very small. With $N_{a m}=80$ we find, for example, that setting $\bar{N}_{a m}=0$ in $\bar{R}_{n}(\ldots)$ (no terms) gives essentially identical results for our quark masses and coupling as setting $\bar{N}_{a m}=30$ (140 terms), even though the latter fit requires 22 times more computing. We used this procedure, with $\bar{N}_{a m}=0$, for most of our testing and development in this project.

## 3. Truncated Perturbation Theory

The perturbative part,

$$
\begin{equation*}
r_{n}\left(\alpha_{\overline{\mathrm{MS}}}, \mu / m_{h}\right)=1+\sum_{j=1}^{N_{\mathrm{pth}}} r_{n j}\left(\mu / m_{h}\right) \alpha_{\overline{\mathrm{MS}}}^{j}(\mu) \tag{20}
\end{equation*}
$$

of the reduced moments is known at best through third order. We present coefficients $r_{n j}$ through $j=3$ in Table III (2-6]; the values for $n=4-10$ are exact, while $r_{n 3}$ is estimated for the others. In our fits we include higherorder terms by treating the coefficients of these terms as fit parameters with prior

$$
\begin{equation*}
r_{n j}(1)=0 \pm 0.5 \tag{21}
\end{equation*}
$$

TABLE III: Perturbation theory coefficients ( $n_{f}=3$ ) for $r_{n}$ [2-6]. Coefficients are defined by $r_{n}=1+\sum_{j=1} r_{n j} \alpha_{\overline{\mathrm{MS}}}^{j}(\mu)$ for $\mu=m_{h}(\mu)$. The third-order coefficients are exact for $4 \leq n \leq 10$. The other coefficients are based upon estimates; we assign conservative errors to these.

| $n$ | $r_{n 1}$ | $r_{n 2}$ | $r_{n 3}$ |
| ---: | ---: | ---: | ---: |
| 4 | 0.7427 | -0.0577 | 0.0591 |
| 6 | 0.6160 | 0.4767 | -0.0527 |
| 8 | 0.3164 | 0.3446 | 0.0634 |
| 10 | 0.1861 | 0.2696 | 0.1238 |
| 12 | 0.1081 | 0.2130 | $0.1(3)$ |
| 14 | 0.0544 | 0.1674 | $0.1(3)$ |
| 16 | 0.0146 | 0.1293 | $0.1(3)$ |
| 18 | -0.0165 | 0.0965 | $0.1(3)$ |

for any coefficient that hasn't been computed in perturbation theory. We set $N_{\text {pth }}=6$ since then contributions from still higher orders should be less than $0.1 \%$ (and setting $N_{\text {pth }}=8$ doesn't change our results).

The perturbative coefficients for $\mu / m_{h}=1$ (Table III) are small and relatively uncorrelated from order-to-order. This is less true for $\mu / m_{h}=3$, which is where we wish to work (see Section II), because of $\log \left(\mu / m_{h}\right)^{m}$ terms. In order to capture these effects, we use renormalization group equations to express the $r_{n j}(3)$ coefficients (for all $j \leq N_{\text {pth }}$ ) in terms of the $r_{n j}(1)$ coefficients and $\log \left(\mu / m_{h}\right)$, and substitute the results from Table III for $j \leq 3$ and from the prior (Eq. (21)) for $j>3$. This procedure generates (correlated) priors for the unknown coefficients at $\mu / m_{h}=3$ that properly account for renormalization-group logarithms.

## 4. $\alpha_{\overline{\mathrm{MS}}}$ Evolution

As discussed above, we fix the ratio of $\mu / m_{h}(\mu)$ in our analysis. This means that the renormalization scale $\mu$ varies over a wide range of values for the different $m_{h} \mathrm{~S}$ we use. The coupling constant $\alpha_{\overline{\mathrm{MS}}}(\mu)$ used in the perturbative expansions for the $r_{n} \mathrm{~s}$ is specified at $\mu=5 \mathrm{GeV}$ by fit parameter $\alpha_{0}$, with prior

$$
\begin{equation*}
\alpha_{0}=0.20 \pm 0.01 \tag{22}
\end{equation*}
$$

where

$$
\begin{equation*}
\alpha_{0} \equiv \alpha_{\overline{\mathrm{MS}}}\left(5 \mathrm{GeV}, n_{f}=3\right) \tag{23}
\end{equation*}
$$

The prior corresponds to $\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}\right)=0.118(3)$ - a very broad range, which means that the prior has little impact on our final fit results. The coupling value at any scale $\mu \neq 5 \mathrm{GeV}$ is obtained by integrating (numerically) the QCD evolution equation for $\alpha_{\overline{\mathrm{MS}}}(\mu)$ starting with value $\alpha_{0}$ at scale 5 GeV . We use the $\overline{\mathrm{MS}}$ beta function
through sixth order in $\alpha_{\overline{\mathrm{MS}}}$,

$$
\begin{align*}
\mu^{2} \frac{d \alpha_{\overline{\mathrm{MS}}}(\mu)}{d \mu^{2}}= & -\beta_{0} \alpha \frac{2}{\overline{\mathrm{MS}}}-\beta_{1} \alpha \frac{3}{\overline{\mathrm{MS}}}-\beta_{2} \alpha \frac{4}{\overline{\mathrm{MS}}}  \tag{24}\\
& -\beta_{3} \alpha \frac{5}{\overline{\mathrm{MS}}}-\beta_{4} \alpha \frac{6}{\overline{\mathrm{MS}}}
\end{align*}
$$

where $\beta_{0} \ldots \beta_{3}$ are known from perturbation theory and $\beta_{4}$ is taken as a fit parameter with prior

$$
\begin{equation*}
\beta_{4}=0 \pm \sigma_{\beta} \tag{25}
\end{equation*}
$$

where $\sigma_{\beta}$ is the root-mean-square average of $\beta_{0} \ldots \beta_{3} 18$, 19]. We include this last term to estimate the uncertainties in our final results caused by unknown terms in the beta function.

Our simulations include vacuum polarization effects from only the three lightest quarks. We use perturbation theory, together with the $c$ and $b$ masses that come out of our analysis, to incorporate vacuum polarization effects from the heavier quarks into our final results for the masses and QCD coupling (using formulas from [20, 21] to add the $c$ and $b$ quarks at scales $\mu=m_{c}$ and $m_{b}$, respectively).

## 5. Nonperturbative Condensates

As discussed in our previous paper, nonperturbative effects dominate the reduced moments when $n$ is large. The dominant nonperturbative contribution, which is from the gluon condensate, is quite small, however, for the range of $n$ s and quark masses we use here. We correct for it by replacing

$$
\begin{equation*}
R_{n}^{\mathrm{latt}} \rightarrow R_{n}^{\mathrm{latt}}\left(1+d_{n} \frac{\left\langle\alpha_{s} G^{2} / \pi\right\rangle}{\left(2 m_{h}\right)^{4}}\right) \tag{26}
\end{equation*}
$$

where $d_{n}$ is computed to leading order in perturbation theory [22] with $m_{h}=m_{h}\left(m_{h}\right)$, which we approximate by $m_{\eta_{h}} / 2.27$. We take

$$
\begin{equation*}
\left\langle\alpha_{s} G^{2} / \pi\right\rangle=0 \pm 0.012 \mathrm{GeV}^{4} \tag{27}
\end{equation*}
$$

which covers the range of most current estimates [23]. The correction factor in Eq. (26) adds (slightly) to the error in $R_{n}^{\text {latt }}$ (and introduces new correlations between different moments, since the same $\left\langle\alpha_{s} G^{2} / \pi\right\rangle$ is assumed for every moment, lattice spacing and quark mass).

## 6. Finite Volume Errors

We expect small errors due to the fact that our simulation lattices are only about 2.5 fm across. We allow for the possibility of finite-volume errors by replacing

$$
\begin{equation*}
R_{n}^{\text {latt }} \rightarrow R_{n}^{\text {latt }}\left(1+f_{n} \frac{\Delta R_{n}^{\text {pth }}}{R_{n}^{\text {pth }}}\right) \tag{28}
\end{equation*}
$$

where $\Delta R_{n}^{\text {pth }}$ is the finite volume error in leading-order perturbation theory and

$$
\begin{equation*}
f_{n}=0 \pm 0.5 \tag{29}
\end{equation*}
$$

The true finite-volume errors are expected to be smaller, because of quark confinement, than the perturbative errors that we use to model them here. We verified this by running two sets of simulations that were identical except for the spatial volume (gluon configuration sets 4 and 5 in Table【I). The differences between the two simulations are smaller than our statistical errors, but the statistical errors are much smaller than our estimate above. Our error estimate here is very conservative, but has negligible impact on our final results.

## 7. Sea-Quark Masses

The sea-quark masses used in our simulations are not exactly correct. To correct for this we replace

$$
\begin{equation*}
R_{n}^{\mathrm{latt}} \rightarrow R_{n}^{\mathrm{latt}}\left(1+g_{n} \frac{2 \delta m_{l}+\delta m_{s}}{m_{s}}\right) \tag{30}
\end{equation*}
$$

where $\delta m_{l}$ and $\delta m_{s}$ are the errors in the $u / d$ and $s$ masses (see 10] for more details), respectively, and

$$
\begin{equation*}
g_{n}=0 \pm 0.01 \tag{31}
\end{equation*}
$$

This correction introduces (correlated) errors into the $R_{n}^{\text {latt }}$ s that are of order $0.5-1 \%$. Direct comparison of results from configuration sets 6 and 7 (or 1-2 and $3-$ 4) in Table $\square$ suggests that sea-quark mass effects are no larger than $0.1 \%$, so our error estimate is conservative.

We have only included the leading dependence on the sea-quark mass, which comes from nonperturbative (chiral) effects. Quadratic terms from perturbation theory and other nonperturbative sources are negligible.

## IV. ANALYSIS AND RESULTS

We have computed reduced moments for 30 different sets of lattice spacing, lattice volume and quark masses (Table III). To extract quark masses and the QCD coupling, we fit moments with $4 \leq n \leq 10$ from 22 of these parameter sets (the ones with $a m_{\eta_{h}} \leq 1.95$ ) - 88 pieces of simulation data in all. In this section we first describe the fitting method used to extract the masses and coupling, and then we review our results.

## A. Constrained Fits

We analyze all four $R_{n}$ s for all 22 parameter sets simultaneously using a constrained fitting procedure based
upon Bayesian ideas [17]. In this procedure we minimize an augmented $\chi^{2}$ function of the form

$$
\begin{equation*}
\chi^{2}=\sum_{i n, j m} \Delta R_{n i}\left(\sigma_{R}^{-2}\right)_{i n, j m} \Delta R_{m j}+\sum_{\xi} \delta \chi_{\xi}^{2} \tag{32}
\end{equation*}
$$

where:

$$
\begin{equation*}
\Delta R_{n i} \equiv R_{n i}^{\text {latt }}-R_{n}\left(\mu_{i}, m_{\eta_{h} i}, a_{i}, N_{a m}\right) ; \tag{33}
\end{equation*}
$$

the $R_{n}^{\text {latt }}$ come from Table II with corrections from Eqs. (26), (28) and (30); fit function $R_{n}(\ldots)$ is defined by Eq. (15); and $\sigma_{R}^{2}$ is the error covariance matrix for the $R_{n}^{\text {latt }}$. The sums $i, j$ are over the 22 sets of lattice spacings and quark masses; the sums $n, m$ range over of the moments $4,6,8,10$.

Function $R_{n}\left(\mu_{i}, m_{\eta_{h} i}, a_{i}, N_{a m}\right)$ depends upon a large number of parameters, all of which are varied in the fit to minimize $\chi^{2}$. Priors $\delta \chi_{\xi}^{2}$ are included for each of these:

- parameters $z_{j}$, with prior Eq. (13), from the $1 / m_{\eta_{h}}$ expansion of $z\left(\mu / m_{h}, m_{\eta_{h}}\right)$;
- parameters $c_{i j}^{(n)}$, with prior Eq. (17), from the finite-lattice spacing corrections;
- unknown perturbative coefficients $r_{n j}$, with prior Eq. (21) (evolved to $\mu / m_{h}=3$ );
- coupling parameter $\log \left(\alpha_{0}\right)$, with prior Eq. (22);
- $\beta_{4}$ in the QCD $\beta$-function, with prior Eq. (25);
- lattice spacings $a_{i}$ for each gluon configuration set, with priors specified by simulation results for $r_{1} / a$ (Table【) and the current value for $r_{1}$ (Eq. (10));
- values for $a m_{\eta_{h} i}$, with priors specified by our simulation results (Table II).

The renormalization scales $\mu_{i}$ are obtained from the ratio $\mu / m_{h}=3$, simulation results for $m_{\eta_{h}}$, and Eq. (7). We take $N_{a m}=30$ for our final results.

## B. Results

We fit our simulation data for the reduced moments $R_{n}^{\text {latt }}$ (Table III) using fit function $R_{n}(\ldots)$ (Eq. (15)) with $N_{a m}=30$, as discussed in the previous section. The best-fit values for parameters $z_{j}$ give us the mass-ratio function $z\left(\mu / m_{h}=3, m_{\eta_{h}}\right)$ (Eq. (7)), which we plot in Figure 1 We also show our simulation results there for $R_{n}^{\text {latt }} / r_{n}$, together with the best-fit lines for each lattice spacing. Results are shown for the three moments that depend upon $z, 5$ different lattice spacings, and quark masses ranging from below the $c$ mass almost to the $b$ mass. The simulation data were all fit simultaneously, using the same functions $z\left(3, m_{\eta_{h}}\right)$ and $\alpha_{\overline{\mathrm{MS}}}(\mu)$ (with $\left.\mu=3 m_{\eta_{h}} /(2 z)\right)$ for all moments. The fits are excellent, with $\chi^{2} / 88=0.19$ for the 88 pieces of simulation data we fit.


FIG. 1: Function $z\left(\mu / m_{h}=3, m_{\eta_{h}}\right) \equiv m_{\eta_{h}} /\left(2 m_{h}\right)$ as a function of $m_{\eta_{h}}$. The solid line, plus gray error envelope, shows the $a=0$ extrapolation obtained from our fit. This is compared with simulation results for $R_{n} / r_{n}$ for $n=6,8,10$ from our 5 different lattice spacings, together with the best fits (dashed lines) corresponding to those lattice spacings. Dashed lines for smaller lattice spacings extend further to the right. The points marked by an " $x$ " are for the largest mass we tried (last line in Table II); these are not included in the fit because $a m_{\eta_{h}}$ is too large. Finite- $a$ errors become very small for the larger- $n$ moments, causing points from different lattice spacings to overlap.

Evaluated at $m_{\eta_{c}}=2.985(3) \mathrm{GeV}$ [24], the massratio function is $z\left(3, m_{\eta_{c}}\right)=1.507(7)$. Combining this with Eq. (9) and perturbation theory, we can obtain the following results for the $\overline{\mathrm{MS}} c$-quark mass at different scales:

$$
\begin{align*}
m_{c}\left(3 m_{c}, n_{f}=3\right) & =0.991(5) \mathrm{GeV},  \tag{34}\\
m_{c}\left(3 \mathrm{GeV}, n_{f}=4\right) & =0.986(6) \mathrm{GeV}, \\
m_{c}\left(m_{c}, n_{f}=4\right) & =1.273(6) \mathrm{GeV} .
\end{align*}
$$

Similarly at $m_{\eta_{b}}=9.395(5) \mathrm{GeV}$ [25], the mass-ratio function is $z\left(3, m_{\eta_{b}}\right)=1.296(8)$, and we obtain the following results for the $\overline{\text { MS }} b$-quark mass at different scales:

$$
\begin{align*}
m_{b}\left(3 m_{b}, n_{f}=3\right) & =3.622(22) \mathrm{GeV} .  \tag{35}\\
m_{b}\left(10 \mathrm{GeV}, n_{f}=5\right) & =3.617(25) \mathrm{GeV}, \\
m_{b}\left(m_{b}, n_{f}=5\right) & =4.164(23) \mathrm{GeV} .
\end{align*}
$$

Note that the ratio $m_{b}\left(\mu, n_{f}\right) / m_{c}\left(\mu, n_{f}\right)$ is independent of $\mu$ and $n_{f}$. We obtain the following result for this


FIG. 2: QCD coupling $\alpha_{\overline{\mathrm{MS}}}\left(\mu, n_{f}=3\right)$ as a function of $m_{\eta_{h}}$ where $\mu=3 m_{h}$. The solid line, plus gray error envelope, shows the best-fit coupling from our fit when perturbative evolution is assumed. The data points are values of $\alpha_{\overline{\text { MS }}}$ extracted from individual simulation results for $R_{n}$ after extrapolating to $a=0$ and dividing out $z\left(3, m_{\eta_{h}}\right)(n>4)$. Results are given for moments $n=4-10$ and all 5 lattice spacings. Several points from different lattice spacings overlap in these plots.
mass ratio:

$$
\begin{equation*}
m_{b} / m_{c}=4.53(4) \tag{36}
\end{equation*}
$$

The other important output from our fit is a value for the parameter

$$
\begin{equation*}
\alpha_{0} \equiv \alpha_{\overline{\mathrm{MS}}}\left(5 \mathrm{GeV}, n_{f}=3\right)=0.2034(21) \tag{37}
\end{equation*}
$$

To compare with other determinations of the coupling, we add vacuum polarization corrections from the $c$ and $b$ quarks, using the masses above, and evolve to the $Z$ meson mass 18 21]:

$$
\begin{equation*}
\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}, n_{f}=5\right)=0.1183(7) \tag{38}
\end{equation*}
$$

TABLE IV: Sources of uncertainty for the QCD coupling and mass determinations in this paper. In each case the uncertainty is given as a percentage of the final value.

|  | $\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}\right)$ | $m_{b}(10)$ | $m_{b} / m_{c}$ | $m_{c}(3)$ |
| :---: | :---: | :---: | :---: | :---: |
| $a^{2}$ extrapolation | $0.2 \%$ | $0.6 \%$ | $0.5 \%$ | $0.2 \%$ |
| perturbation theory | 0.5 | 0.1 | 0.5 | 0.4 |
| statistical errors | 0.1 | 0.3 | 0.3 | 0.2 |
| $m_{h}$ extrapolation | 0.1 | 0.1 | 0.2 | 0.0 |
| errors in $r_{1}$ | 0.2 | 0.1 | 0.1 | 0.1 |
| errors in $r_{1} / a$ | 0.1 | 0.3 | 0.2 | 0.1 |
| errors in $m_{\eta_{c}}, m_{\eta_{b}}$ | 0.2 | 0.1 | 0.2 | 0.0 |
| $\alpha_{0}$ prior | 0.1 | 0.1 | 0.1 | 0.1 |
| gluon condensate | 0.0 | 0.0 | 0.0 | 0.2 |
| Total | $0.6 \%$ | $0.7 \%$ | $0.8 \%$ | $0.6 \%$ |

Figure 2 shows how consistent our simulation results are with the theoretical curve for $\alpha_{\overline{\mathrm{MS}}}\left(\mu, n_{f}=3\right)$ corresponding to our value for $\alpha_{0}$. For this figure we extracted values for $\alpha_{\overline{\mathrm{MS}}}$ from each $R_{n}$ separately by dividing out the $a^{2}$ dependence and $z\left(3, m_{\eta_{h}}\right)$ using our best-fit parameters, and then solving for $\alpha_{\overline{\mathrm{MS}}}$ by matching with perturbation theory for $r_{n}$. (In our fit, of course, we fit all $R_{n} \mathrm{~S}$ simultaneously to obtain a single $\alpha_{\overline{\mathrm{MS}}}$ for all of them.)

The dominant sources of error for our results are listed in Table IV. The largest uncertainties come from: extrapolations to $a=0$, especially for quantities involving $b$ quarks; unknown higher-order terms in perturbation theory, especially for quantities involving $c$ quarks; statistical fluctuations; extrapolations in the heavy quark mass, especially for quantities involving $b$ quarks; and uncertainties in static-quark parameters $r_{1} / a$ and $r_{1}$. The pattern of errors is as expected in each case. The nonperturbative contribution from the gluon condensate is negligible except for $m_{c}$, again as expected; and errors due to mistuned sea-quark masses, finite volume errors, and uncertainties in $\overline{\mathrm{MS}}$ coupling and mass evolution are negligible ( $<0.05 \%$ ).

The $a^{2}$ extrapolations of our data are not large. This is illustrated for $m_{h} \approx m_{c}$ in Figure 3, which shows the $a^{2}$ dependence of the reduced moments. The smallest two lattice spacings are sufficiently close to $a=0$ that the extrapolation is almost linear from those points. The $a=$ 0 extrapolated values we obtain here for the $R_{n}$ agree to within (smaller) errors with those in our previous paper: here we get $1.282(4), 1.527(4), 1.373(3), 1.304(2)$ with $n=4,6,8,10$, respectively, for the masses used in the figure.

We tested the stability of our analysis in several ways:

- Vary perturbation theory: We chose $\mu=3 m_{h}$ in order to keep scales large and $\alpha_{\overline{\mathrm{MS}}}(\mu)$ small. Our results are quite insensitive to $\mu$, however. Choosing $\mu=m_{h}$, for example, shifts none of our results by more than $0.2 \sigma$, and leaves all errors unchanged except for $m_{c}(3)$, where the error increases by a third. Taking $\mu=9 m_{h}$ shifts results by less than


FIG. 3: Lattice spacing dependence of $R_{n}$ for masses $m_{\eta_{h}}$ within $5 \%$ of $m_{\eta_{c}}$ and moments $n=4,6,8,10$. The dashed lines show our fit for the average of these masses, and the points at $a=0$ are the continuum extrapolations of our data.
$0.4 \sigma$, and reduces the $m_{c}$ error by a third, leaving others only slightly reduced. Adding more terms to the perturbative expansions $\left(N_{\text {pth }}=6 \rightarrow 8\right)$ also has essentially no effect on the results. The prior for the unknown perturbative coefficients (Eq. (21)) is twice as wide as suggested by our simulation results (using the empirical Bayes criterion [17]); we choose the larger width to be conservative.

- Include more/fewer finite-a corrections: We set $N_{a m}=30$ for our results above. Using $N_{a m}=15$ gives results that differ by less than $0.5 \sigma$ for $m_{b}$ and much less for the other quantities. Much larger $N_{a m} \mathrm{~s}$ can be tested easily using the trick described in Section IIIB 2, For example, replacing $R_{n}^{\text {latt }}$ by $\bar{R}_{n}^{\text {latt }}$ (Eq. (18)) with $N_{a m}=80$ and $\bar{N}_{a m}=30$ gives results that are essentially identical to those above. As discussed above, taking $\bar{N}_{a m}=0$ with the same $N_{a m}$ also gives the same results and is 22 times faster (see the appendix for further discussion).
- Change $n$ dependence of finite-a corrections: Replacing the $n$-dependent prior for the expansion coefficients (Eq. (17)) by the $n$-independent prior $0 \pm$ 0.5 causes changes that are less than $0.3 \sigma$. The width of the original prior is optimal according to the empirical Bayes criterion - that is, it is the width suggested by the size of finite- $a$ deviations observed in our simulation data.
- Add more/fewer $\Lambda / m \eta_{h}$ terms in $z$ : Increasing the number of terms in the expansion for $z$ from $N_{z}=4$ to 6 changes nothing by more than $0.1 \sigma$. Decreasing to $N_{z}=3$ also has no effect. Again the width of the prior is optimal according to the empirical Bayes criterion.
- Include more/fewer moments: Keeping all mo-
ments $4 \leq n \leq 18$ changes nothing by more than $0.5 \sigma$ and reduces errors slightly for everything other than $m_{b}$, where the errors are cut almost in half: $m_{b}(10)=3.623(15) \mathrm{GeV}$ or $m_{b}\left(m_{b}\right)=$ $4.170(13) \mathrm{GeV}$, both for $n_{f}=5$. We continue to restrict ourselves to moments with $n \leq 10$ because these are the only moments for which we have exact third-order perturbation theory. Keeping just $n=4,6$ gives almost identical results for $m_{c}$ and $\alpha_{\overline{\mathrm{MS}}}$, with almost the same errors, but doubles the error on $m_{b}$.
- Omit simulation data: The coarsest two lattice spacings (configuration sets $1-5$ ) affect our results only weakly. Leaving these out shifts no result by more than $0.5 \sigma$ and leaves errors almost unchanged. Leaving out the smallest lattice spacing, however, increases errors significantly (almost double for $\alpha_{\overline{\mathrm{MS}}}$ ), while still shifting central values by less than $0.5 \sigma$.
- Add large masses: Including cases with $a m_{\eta_{h}}>$ 1.95 from Table II leads to poor fits. The excluded data, however, do not deviate far from the best-fit lines. For example, the points marked with an " $x$ " in Figure 1 are for the largest mass we studied, corresponding to $m_{\eta_{h}}=9.15 \mathrm{GeV}$ (last line in Table III). Although $a m_{\eta_{h}}$ is too large for this case to be included in our fit, the values of $R_{n} / r_{n}$ are only slightly below the fit results.


## V. NONPERTURBATIVE $m_{b} / m_{c}$

It is possible to extract the ratio of quark masses $m_{b} / m_{c}$ directly, without using the moments and without using perturbation theory. This provides an excellent nonperturbative check on our results from the moments.

Ratios of quark masses are UV-cutoff independent and therefore the ratio of $\overline{\mathrm{MS}}$ masses

$$
\begin{equation*}
\frac{m_{b}\left(\mu, n_{f}\right)}{m_{c}\left(\mu, n_{f}\right)}=\frac{m_{0 b}}{m_{0 c}}+\mathcal{O}\left(\alpha_{s} a^{2} m_{b}^{2}\right) \tag{39}
\end{equation*}
$$

for any $\mu$ and $n_{f}$, where $m_{0 b}$ and $m_{0 c}$ are the bare quark masses in the lattice quark action that give correct masses for the $\eta_{c}$ and $\eta_{b}$, respectively. We obtain accurate mass ratios from this relationship by extrapolating to $a=0$. We used such a method recently to determine $m_{c} / m_{s}$ [11].

Here we have to modify our earlier method slightly because we cannot reach the $b$-quark mass directly, but rather must simultaneously extrapolate to the $b$ mass and the continuum limit. This is most simply done by determining the functional dependence of the ratio

$$
\begin{equation*}
w\left(m_{\eta_{h}}, a\right) \equiv \frac{2 m_{0 h}}{m_{\eta_{h}}} \tag{40}
\end{equation*}
$$

on the $\eta_{h}$ mass and the lattice spacing. The ratio of $\overline{\mathrm{MS}}$ masses is then given by the experimental masses of the $\eta_{c}$ and $\eta_{b}$ and the equation:

$$
\begin{equation*}
\frac{m_{b}\left(\mu, n_{f}\right)}{m_{c}\left(\mu, n_{f}\right)}=\frac{m_{\eta_{b}}^{\exp } w\left(m_{\eta_{b}}^{\exp }, 0\right)}{m_{\eta_{c}}^{\exp } w\left(m_{\eta_{c}}^{\exp }, 0\right)} \tag{41}
\end{equation*}
$$

It might seem simpler to fit $m_{0 h}$ directly, rather than the ratio $w$; but using $w$ significantly reduces the $m_{\eta_{h}}$ dependence (and therefore our extrapolation errors), and also makes our results quite insensitive to uncertainties in our values for the lattice spacing.

We parameterize function $w$ with an expansion modeled after the one we used to fit the moments:

$$
\begin{align*}
& w\left(m_{\eta_{h}}, a\right)=Z_{m}(a)\left(1+\sum_{n=1}^{N_{w}} w_{n}\left(\frac{2 \Lambda}{m_{\eta_{h}}}\right)^{n}\right) /  \tag{42}\\
&\left(1+\sum_{i=1}^{N_{a m}} \sum_{j=0}^{N_{w}} c_{i j}\left(\frac{a m_{\eta_{h}}}{2}\right)^{2 i}\left(\frac{2 \Lambda}{m_{\eta_{h}}}\right)^{j}\right)
\end{align*}
$$

where, as for the moments,

$$
\begin{equation*}
i+j \leq \max \left(N_{a m}, N_{w}\right) \tag{43}
\end{equation*}
$$

Coefficients $c_{i j}$ and $w_{n}$ are determined by fitting function $w\left(m_{\eta_{h}}, a\right)$ to the values of $2 a m_{0 h} /\left(a m_{\eta_{h}}\right)$ from Table II. The fit also determines the parameters $Z_{m}(a)$, one for each lattice spacing, which account for the running of the bare quark masses between different lattice spacings.

The finite- $a$ dependence is smaller here than for the moments, because the $\eta_{h}$ is nonrelativistic (finite- $a$ errors are suppressed by additional powers of $v / c$ [8]), and the variation with $m_{\eta_{h}}$ stronger (twice that of $z\left(3, m_{\eta_{h}}\right)$ ). So here we use priors

$$
\begin{align*}
c_{i j} & =0 \pm 0.05  \tag{44}\\
w_{n} & =0 \pm 4 \\
Z_{m}(a) & =1 \pm 0.5
\end{align*}
$$

with $N_{w}=8$. We again take $N_{a m}=30$, although identical results are obtained with $N_{a m}=15$.

Our fit results are illustrated by Figure 4 which plots the ratio $m_{0 h} / m_{\eta_{h}}$ divided by $m_{0 c} / m_{\eta_{c}}$ for a range of $\eta_{h}$ masses. Our data for different lattice spacings is compared with our fit, and with the $a=0$ limit of our fit (solid line). The fit is excellent, with $\chi^{2} / 22=0.42$ for the 22 pieces of data we fit (we again exclude cases with $\left.a m_{\eta_{h}}>1.95\right)$. Using the $\eta_{c}$ and $\eta_{b}$ masses from Section IVB, and Eq. (41) with the best-fit values for the parameters, we obtain finally

$$
\begin{align*}
\frac{m_{0 b}}{m_{0 c}} & \rightarrow 4.49(4) \quad \text { as } a \rightarrow 0  \tag{45}\\
& =\frac{m_{b}\left(\mu, n_{f}\right)}{m_{c}\left(\mu, n_{f}\right)}
\end{align*}
$$

which agrees well with our result from the moments (Eq. (36) ).


FIG. 4: Ratio $m_{0 h} / m_{\eta_{h}}$ divided by $m_{0 c} / m_{\eta_{c}}$ (which we approximate by $w\left(m_{\eta_{c}}, a\right) / 2$ from our fit) as a function of $m_{\eta_{h}}$. The solid line shows the $a=0$ extrapolation obtained from our fit. This is compared with simulation results for our 4 smallest lattice spacings, together with the best fits (dashed lines) corresponding to those lattice spacings. The point marked by an " $x$ " is for the largest mass we tried (last line in Table 【I); this was not included in the fit because $a m_{\eta_{h}}$ is too large.

## VI. $\alpha_{\overline{\text { MS }}}$ FROM WILSON LOOPS

In a recent paper [26], we presented a very accurate determination of the QCD coupling from simulation results for Wilson loops. Here we want to compare those results to the value we obtain from heavy-quark correlators. First, however, we must update our earlier analysis to take account of the new value for $r_{1}$ [10] given in Eq. (10) and improved values for $r_{1} / a$ (13] given in Table (The Wilson-loop paper uses some additional configuration sets: from Table II in that paper, sets $1,6,9$, and 11 whose new $r_{1} / a$ s are 1.813(8), 2.644(3), 5.281(8) and $5.283(8)$, respectively.) We have rerun our earlier analysis, updating $r_{1}, r_{1} / a$, and the $c$ and $b$ masses. The results are shown in Figure 5. Combining results as in the earlier paper we obtain a final value from the Wilson-loop quantities of

$$
\begin{equation*}
\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}, n_{f}=5\right)=0.1184(6), \tag{46}
\end{equation*}
$$

with $\chi^{2} / 22=0.3$ for the 22 quantities in the figure. This agrees very well with the result in the earlier paper, $\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}\right)=0.1183(8)$, but has a slightly smaller error, as expected given the smaller error in $r_{1}$. This new value also agrees well with our very different determination from heavy-quark correlators (Eq. (38)). A breakdown of the error into its different sources can be found in Table IV of [26] (reduce the $r_{1}$ and $r_{1} / a$ errors in that table by half to account for the improved values used here).


FIG. 5: Updated values for the 5 -flavor $\alpha_{\overline{\mathrm{MS}}}$ at the $Z$-meson mass from each of 22 different short-distance quantities built from Wilson loops. The gray band indicates a composite average, $0.1184(6) . \chi^{2}$ per data point is 0.3 .

## VII. CONCLUSIONS

In this paper, we improve significantly on our previous determinations of the QCD coupling and $c$-quark mass from heavy-quark correlators. This is principally due to the inclusion of a new, smaller lattice spacing in our analysis. We also generated results for a variety of quark masses near $m_{c}$, allowing us to interpolate more accurately to the physical value of $m_{c}$. New third-order perturbation theory makes $R_{10}$ as useful now as $R_{4}, R_{6}$, and $R_{8}$ were in the earlier paper. Finally, in this paper, we fit multiple moments simultaneously, determining consistent values simultaneously for both the QCD coupling and the quark masses for all moments. Previously we examined each moment or ratio of moments independently, extracting $m_{c}$ s or $\alpha_{\overline{\mathrm{MS}}} \mathrm{s}$ independently of each other. Our


FIG. 6: $z\left(\mu / m_{h}, m_{\eta_{h}}\right)$ versus $m_{\eta_{h}}$ (in GeV ) for three different values of $\mu / m_{h}$. The curve for $\mu=3 m_{h}$ comes from the best fit to the moments. The other curves are obtained by evolving perturbatively from $\mu=3 m_{h}$.


FIG. 7: Simulation results for reduced moments $R_{n}$ with $n=$ $6,8,10$ as functions of $m_{\eta_{h}}$ for 5 different lattice spacings. The dashed lines show the corresponding behavior of our fit function, with the best-fit parameters. The curves for smaller lattice spacings extend further to the right. The solid lines show the $a=0$ limit of our best fit.
new results,

$$
\begin{align*}
m_{c}\left(3 \mathrm{GeV}, n_{f}\right. & =4)  \tag{47}\\
\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}, n_{f}\right. & =5)
\end{align*}=0.986(6) \mathrm{GeV}, 1183(7), ~ \$
$$

agree well with our older results of $0.986(10) \mathrm{GeV}$ and $0.1174(12)$, respectively [1].

The much heavier $b$ quark is usually analyzed using effective field theories like NRQCD or the static-quark approximation. By using very small lattice spacings and the very highly improved HISQ discretization for the heavy quarks, we are able to extend our analysis almost to the $b$-quark mass, using the same relativistic discretization that we use for $c$ and lighter quarks. A $1.5 \%$ extrapolation of $z\left(3, m_{h}\right)$, from the largest $m_{\eta_{h}}$ used in our fits to $m_{\eta_{b}}$, gives us a new, accurate determination of the $b$-quark mass,

$$
\begin{equation*}
m_{b}\left(10 \mathrm{GeV}, n_{f}=5\right)=3.617(25) \mathrm{GeV} \tag{48}
\end{equation*}
$$

This calculation demonstrates the utility of the HISQ formalism for studying $b$ quarks on lattices that are computationally accessible today. This represents a breakthrough for $b$ physics on the lattice since far greater precision becomes possible when all quarks are treated using the same formalism, and that formalism is relativistic and has a chiral symmetry. Even better would be to work right at the $b$ mass, as opposed to extrapolating from nearby; this would require a lattice spacing of order 0.03 fm .

Both of our new $c$ and $b$ masses agree well with non-lattice determinations from vector-current correlators and experimental $e^{+} e^{-}$collisions. A recent analysis of the continuum data gives [7]

$$
\begin{align*}
m_{c}\left(3 \mathrm{GeV}, n_{f}\right. & =4) \tag{49}
\end{align*}=0.986(13) \mathrm{GeV},{ }_{b}\left(m_{b}, n_{f}=5\right)=4.163(16) \mathrm{GeV}
$$

which compare well with our values of $0.986(6) \mathrm{GeV}$ and $4.164(23) \mathrm{GeV}$, respectively. This provides strong evidence that the different systematic errors in each calculation are understood.

Function $z\left(\mu / m_{h}, m_{\eta_{h}}\right)$ is a by-product of our analysis. It relates the $\overline{\mathrm{MS}}$ quark mass $m_{h}(\mu)$ to the $\eta_{h}$ mass (Eq. (7)). We show our result again in Figure 6 for $\mu=3 m_{h}$, as well as for $\mu=m_{h}$ and $\mu=m_{h} / 2$, which we obtain by evolving perturbatively from $\mu=3 m_{h}$. The latter two curves are relatively flat, and the last surprisingly close to 1 for most masses.

Questions have been raised about the way perturbation theory is used in analyzing the perturbative parts of the moments [27]. Like 7] we favor using larger scales than $m_{c}$ for $c$-quark correlators, but, as we have shown, our results are quite insensitive to $\mu$ over a broad range. Furthermore, the fact that our results, from pseudoscalar-density correlators, agree so well with the continuum results, from vector-current correlators, is also compelling evidence that perturbation theory is being handled correctly. We also find consistent results from several different moments, which is only possible if perturbation theory is working well. Compare, for example, Figure 7 for the moments, as a function of $m_{\eta_{h}}$, with the plots of $R_{n} / r_{n}$ in Figure 1 Figure 7 shows very different $m_{\eta_{h}}$ behavior, at the 10-20\% level, for different moments $R_{n}$; Figure 1, where the perturbative part $r_{n}$ is divided out, shows behavior that is almost momentindependent.

An additional check on our use of perturbation theory comes from the close agreement between our perturbative result for the ratio $m_{b} / m_{c}$ of $\overline{\mathrm{MS}}$ masses (Eq. (36)) and our nonperturbative result for the ratio of HISQ masses (Eq. (45)). These should be and are equal to within our 1\% errors. Taken together they suggest a composite result of:

$$
\begin{equation*}
\frac{m_{b}\left(\mu, n_{f}\right)}{m_{c}\left(\mu, n_{f}\right)}=4.51(4) \quad \text { (composite). } \tag{50}
\end{equation*}
$$

The validity of our perturbative analyses is further supported by the close agreement between the


FIG. 8: The 5 -flavor QCD coupling $\alpha_{\overline{\text { MS }}}$ at the $Z$ mass as determined by a variety of different methods. The non-lattice numbers used here are from the review in [28].

QCD coupling we get from the heavy-quark correlators, $\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}\right)=0.1183(7)$, and that obtained from Wilson loops, $0.1184(6)$. These are radically different methods for determining the coupling. The first relies upon a continuum quantity, extrapolated to $a=0$, and continuum perturbation theory. The second relies upon quantities that are highly sensitive to the UV cutoff $(\pi / a)$ but are analyzed to all orders in the cutoff using lattice perturbation theory. Systematic errors are almost completely different in the two cases. The fact that they agree to within our $0.6 \%$ uncertainties is highly nontrivial evidence that perturbative and other potential errors are understood.

Our coupling values also agree well with determinations from non-lattice methods. Figure 8 summarises recent results that were included in a world average by Bethke [28]. The world average result, 0.1184(7), was dominated by our previous determination from the Wilson loop analysis. The average excluding our result was 0.1186(11), which also agrees well. Including our new results into a new error-weighted world average gives $\alpha_{\overline{\mathrm{MS}}}\left(M_{Z}\right)=0.1184(4)$.

Our new $c$ mass is the most accurate currently available. With it we can improve slightly on our recent determination of light quark masses using an accurate value for $m_{c} / m_{s}, 11.85(16)$, derived completely nonperturbatively from lattice calculations [11]. Our new $c$ mass, which becomes $1.093(6) \mathrm{GeV}$ when converted to $n_{f}=3$ at 2 GeV , implies:

$$
\begin{align*}
& m_{s}\left(2 \mathrm{GeV}, n_{f}=3\right)=92.2(1.3) \mathrm{MeV}  \tag{51}\\
& m_{d}\left(2 \mathrm{GeV}, n_{f}=3\right)=4.77(15) \mathrm{MeV} \\
& m_{u}\left(2 \mathrm{GeV}, n_{f}=3\right)=2.01(10) \mathrm{MeV}
\end{align*}
$$

Our results for all 5 quark masses are compared with the


FIG. 9: $\overline{\mathrm{MS}}$ masses, for the 5 lightest quarks, from this paper compared with the Particle Data Group's current estimates 29]. Each mass is quoted at its conventional scale: 2 GeV for $u, d, s\left(n_{f}=3\right) ; m_{c}$ for $c\left(n_{f}=4\right) ; m_{b}$ for $b\left(n_{f}=5\right)$.

Particle Data Group's 2009 values in Figure 9 . Agreement is excellent, but our uncertainties are much smaller in every case, and by an order of magnitude for the strange and light quarks.

Finally we note that the consistency between quark masses from lattice and non-lattice analyses, and between couplings from heavy-quark correlators and Wilson loops provides further evidence that taste-changing interactions in the HISQ and ASQTAD quark formalisms are understood and vanish as $a \rightarrow 0$. While early concerns about the validity of these formalisms have been largely addressed both by formal arguments [13, 30-34] and by extensive empirical studies 8-11, 26, 35-39], it remains important to test the simulation technology of lattice QCD with increasing precision, given the growing importance of lattice results for phenomenology.

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## Appendix: Accelerated Fitting

In Section III B 2 we used a trick to simplify our fits by, in effect, transferring fit terms from the fit function into the errors of the fit data. This trick can greatly speed up complicated fits. Here we present a formal derivation of this procedure for three increasingly complicated situations.

## A. Linear Least Squares - Exact Data

Assuming we know $D$ values $y_{i}$ for a quantity $y$ which can be expressed as a power series in $x$,

$$
\begin{equation*}
y=\sum_{n} c_{n} x^{n} \tag{52}
\end{equation*}
$$

we wish to obtain a best fit for the first $F$ unknown coefficients $c_{n}$. The $c_{n}$ are then our random variables. If we are able to make reasonable estimates for their means and standard deviations $\sigma_{n}$, in the absence of additional information, maximizing entropy suggests a Gaussian prior of

$$
\begin{equation*}
P(c) \propto e^{-\sum_{n} c_{n}^{2} / 2 \sigma_{n}^{2}} \tag{53}
\end{equation*}
$$

For simplicity, we assume throughout that the $c_{n}$ are uncorrelated and have a prior mean of zero; extending to more general cases is straightforward.

If we knew all coefficient values, then the data $y_{i}$ would be completely determined, with

$$
\begin{equation*}
P(y \mid c) \propto \prod_{i=0}^{D-1} \delta\left(y_{i}-\sum_{n} c_{n} x_{i}^{n}\right) \tag{54}
\end{equation*}
$$

Bayes' theorem

$$
\begin{equation*}
P(c \mid y) \propto P(y \mid c) P(c) \tag{55}
\end{equation*}
$$

allows us to convert this into a distribution for $c$ given the data $y$.

If we are only interested in fitting a subset of coefficients $c_{n_{<}}$with $n<F$, we integrate over the remaining $c_{n_{>}}$, giving

$$
\begin{align*}
P\left(c_{<} \mid y\right) & \propto e^{-\sum_{n_{<}} c_{n<}^{2} / 2 \sigma_{n}^{2}} \times  \tag{56}\\
& {\left[\int d c_{>} \delta^{D}\left(y-\sum_{n} c_{n} x^{n}\right) e^{-\sum_{n>} c_{n>}^{2} / 2 \sigma_{n}^{2}}\right] . }
\end{align*}
$$

We replace the delta function by its Fourier representation, integrate over first the $c_{n_{>}}$, then the Fourier variables, to obtain

$$
\begin{align*}
P\left(c_{<} \mid y\right) & \propto e^{-\sum_{n_{<}} c_{n_{<}}^{2} / 2 \sigma_{n}^{2}} \times  \tag{57}\\
& \left(\operatorname{det} \sigma_{\Delta}^{2}\right)^{-1 / 2} e^{-\Delta y \cdot\left(2 \sigma_{\Delta}^{2}\right)^{-1} \cdot \Delta y}
\end{align*}
$$

Here

$$
\begin{equation*}
\Delta y_{i} \equiv y_{i}-\sum_{n_{<}} c_{n_{<}} x_{i}^{n} \tag{58}
\end{equation*}
$$

is the discrepancy between the measured $y_{i}$ and the portion of the series to be kept in the fit, the dot product sums over the $D$ data points, and

$$
\begin{equation*}
\sigma_{\Delta i j}^{2} \equiv \sum_{n>} x_{i}^{n} \sigma_{n}^{2} x_{j}^{n} \tag{59}
\end{equation*}
$$

The correlation matrix $\sigma_{\Delta}^{2}$ is independent of $c_{<}$(so the determinant is constant), and is the same as one would compute directly by

$$
\begin{equation*}
\left\langle\Delta y_{i} \Delta y_{j}\right\rangle_{c_{>}}=\left\langle\sum_{m_{>}} c_{m>} x_{i}^{m} \sum_{n_{>}} c_{n>} x_{j}^{n}\right\rangle_{c_{>}} \tag{60}
\end{equation*}
$$

using

$$
\begin{equation*}
\left\langle c_{m>} c_{n>}\right\rangle_{c_{>}}=\sigma_{n}^{2} \delta_{m n} \tag{61}
\end{equation*}
$$

Finally, we fit $c_{<}$by minimizing $\chi^{2}$, which includes these correlations and is augmented by the remaining $c_{<}$priors. Because the distribution is Gaussian, the $c_{<}$at their minima are equal to their average values.

The correlation matrix $\sigma_{\Delta}^{2}$ properly accounts for correlations in the discrepancy, due to the neglected terms, between $y$ and the portion of the series retained. If $F$ terms are kept in the series, $\sigma_{\Delta}$ is $\mathcal{O}\left(x^{F}\right)$, enforcing agreement between $y$ and the finite series to this order, as appropriate. It also suggests an alternative but equivalent approach. We may define new random (rather than exact) versions of $y$, whose correlation matrix is $\sigma_{\Delta}^{2}$, by moving the $c_{>}$terms to the left side of Eq. (52). Using the truncated series as a model for these random data, straightforward application of Bayes' theorem [17] again implies the distribution in Eq. (57).

One useful consequence is that, as long as we include the correlations for the $c_{>}$, we may arbitrarily reduce the number of coefficients $c_{<}$retained, even to as few as one, and still obtain the same minimization values. To see this, note that to compute a particular $\left\langle c_{n_{<}}\right\rangle$, we could start with the full distribution and integrate over all $c s$. The integral over $c_{>}$produces $P\left(c_{<} \mid y\right)$, which we then use in the integral over $c_{<}$; the result will be the same regardless of where the dividing line is set, as long as it does not include $c_{n_{<}}$. (We could even include in $\sigma_{\Delta}^{2}$ terms of order less than $n$.) Because averaging and minimization give the same result, the minimization value for $c_{n_{<}}$will also remain unchanged. This is also true of the $c_{n_{<}}$error. While the result is the same, reducing the number of terms in the series to fit can significantly improve the fitting time.

## B. Fits to Nonlinear Functions - Exact Data

We now consider fitting to the data $y_{i}$ a general function $g_{i}\left(c_{n}\right)$ not necessarily linear in the parameters $c$, and
where we assume $y_{i}=g_{i}\left(c_{n}\right)$ exactly for properly chosen $c_{n}$. Now

$$
\begin{equation*}
P(y \mid c) \propto \prod_{i=0}^{D-1} \delta\left(y_{i}-\sum_{n} g_{i}\left(c_{n}\right)\right) \tag{62}
\end{equation*}
$$

Combining with the prior $P(c)$ and integrating over the $c_{>}$gives $P\left(c_{<} \mid y\right)$.

If our estimate of prior means is good, expanding $g$ around $c_{>}=0$ should give a reasonable approximation; an expansion to first order gives a Gaussian. More specifically, defining

$$
\begin{equation*}
g_{i}\left(c_{<}\right) \equiv g_{i}\left(c_{<}, c_{>}=0\right) \tag{63}
\end{equation*}
$$

and

$$
\begin{equation*}
\Delta y_{i} \equiv y_{i}-g_{i}\left(c_{<}\right) \tag{64}
\end{equation*}
$$

and integrating over $c_{>}$in this Gaussian approximation gives as before

$$
\begin{align*}
P\left(c_{<} \mid y\right) & \propto e^{-\sum_{n<} c_{n<}^{2} / 2 \sigma_{n}^{2}} \times  \tag{65}\\
& \left(\operatorname{det} \sigma_{\Delta}^{2}\left(c_{<}\right)\right)^{-1 / 2} e^{-\Delta y \cdot\left(2 \sigma_{\Delta}^{2}\left(c_{<}\right)\right)^{-1} \cdot \Delta y}
\end{align*}
$$

but with

$$
\begin{equation*}
\sigma_{\Delta}^{2}\left(c_{<}\right)_{i j} \equiv \sum_{n>} \partial_{n} g_{i}\left(c_{<}\right) \sigma_{n}^{2} \partial_{n} g_{j}\left(c_{<}\right) \tag{66}
\end{equation*}
$$

This is again the correlation one would compute directly for $\left\langle\Delta y_{i} \Delta y_{j}\right\rangle_{c>}$ after expanding $g$ to first order in $c_{>}$.

We have not expanded in $c_{<}$, so $\sigma_{\Delta}^{2}$ depends on $c_{<}$, the determinant in front is not constant, and the dependence of $\Delta y$ on $c_{<}$is not in general linear. In practice, however, we will often further approximate the distribution by setting the $c_{<}$to their prior means in $\sigma_{\Delta}^{2}\left(c_{<}\right)$before minimization.

Because $g\left(c_{<}\right)$is nonlinear, $c_{<}$from minimization can differ slightly from $\left\langle c_{<}\right\rangle$, and due to approximations made, can vary somewhat with the number of terms retained.

## C. Fits to Data with Intrinsic Statistical Errors

Finally we consider the most general case, in which the data $y$ contribute intrinsic statistical uncertainties in addition to those associated with the truncated series. If we measure a range of values for $y$ with an average $\langle y\rangle$ and correlation matrix $\sigma_{y}^{2}$, then for sufficiently large samples we expect a Gaussian distribution

$$
\begin{equation*}
P(\langle y\rangle \mid c) \propto e^{-(\langle y\rangle-g(c)) \cdot\left(2 \sigma_{y}^{2}\right)^{-1} \cdot(\langle y\rangle-g(c))} \tag{67}
\end{equation*}
$$

rather than the delta function above. Combining with the prior $P(c)$ gives $P(c \mid\langle y\rangle)$.

Expanding $g_{i}\left(c_{<}, c_{>}\right)$to first order around $c_{>}=0$, defining

$$
\begin{equation*}
\Delta y_{i} \equiv\left\langle y_{i}\right\rangle-g_{i}\left(c_{<}\right) \tag{68}
\end{equation*}
$$

and integrating $P(c \mid\langle y\rangle)$ over $c_{>}$gives

$$
\begin{align*}
P\left(c_{<} \mid\langle y\rangle\right) & \propto e^{-\sum_{n<} c_{n<}^{2} / 2 \sigma_{n}^{2}} \times  \tag{69}\\
& \left(\operatorname{det} \sigma_{y \Delta}^{2}\left(c_{<}\right)\right)^{-1 / 2} e^{-\Delta y \cdot\left(2 \sigma_{y \Delta}^{2}\left(c_{<}\right)\right)^{-1} \cdot \Delta y}
\end{align*}
$$

The resulting correlation matrix is a combination of true statistical and neglected series contributions, with

$$
\begin{equation*}
\sigma_{y \Delta}^{2}\left(c_{<}\right) \equiv \sigma_{y}^{2}+\sigma_{\Delta}^{2}\left(c_{<}\right) \tag{70}
\end{equation*}
$$

as one would obtain by including both sources of uncertainty in computing $\left\langle\Delta y_{i} \Delta y_{j}\right\rangle$ directly. With no statistical fluctuations in $y, \sigma_{y}^{2}=0$, and it reduces to the previous result. When $\sigma_{y}^{2}$ is nonzero but small, $\sigma_{\Delta}^{2}$ still makes an important contribution.

## D. Application to this Paper

We used the technique described here in much of our testing and tuning (but not for our final results) to speed up the $\left(a m_{\eta_{h}} / 2\right)^{2}$ fit. As described in Section III B 2, we kept corrections through order $N_{a m}=80$ but moved all but $\bar{N}_{a m} \ll N_{a m}$ out of the fit function and into the errors for the reduced moments. If we set $\bar{N}_{a m}=3$, for example, our fit to the $R_{n}$ simulation data changes from Figure 7 to Figure 10. The small $\bar{N}_{a m}$ means that each point in Figure 10 has much larger error bars, coming from $\left(a m_{\eta_{h}} / 2\right)^{2}$ terms moved into the $R_{n}$ s. The final fit results, however, are almost identical in both cases (to within less than $0.1 \sigma$ ), with the same errors. Note that the $R_{n}$ errors in Figure 10 are highly correlated, which is why the fit curve passes through the central value for each point. As discussed above these correlations are essential if results are to be independent of the value of $\bar{N}_{a m}$.
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FIG. 10: Same as Figure 7 but with $N_{a m}=80$ and $\bar{N}_{a m}=3$, instead of $N_{a m}=\bar{N}_{a m}=30$. The error bars are almost entirely due to systematic errors caused by $a m_{\eta_{h}} / 2$ corrections omitted from the fit function.

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# Heavy-light current-current correlators 

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The current-current correlator method has been used successfully to obtain very accurate results for quark masses and the coupling $\alpha_{s}$. The calculations were done using Highly Improved Staggered Quarks (HISQ) and heavy-heavy meson correlators. We now extend this work to the significantly more challenging heavy-light case, reporting the first results here. The aim is to determine nonperturbative $Z$ factors for NRQCD heavy-light currents, but first we test the method in the HISQ case where $Z=1$.

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[^297]
## 1. Motivation

In the study of semileptonic and leptonic processes, like $B \rightarrow \pi l v$ and $B \rightarrow l v$, the nonperturbative $Z$ factors for heavy-light currents are needed. One way to try to calculate these (nonperturbatively on the lattice) is the current-current correlator method, that has been successfully tested and used in the heavyonium case [ [ ] , $]$. We now want to extend these results and use the same method in the heavy-light case. Here we report on the first results using the HISQ action. The eventual aim is to extract NRQCD heavy-light $Z$ factors.

## 2. Current-current correlator method

The idea is to match time moments of meson correlators to energy-derivative moments at $q^{2}=0$ of polarization functions $\Pi$ calculated in continuum QCD perturbation theory to high order.

The pseudoscalar current-current correlators are defined as

$$
\begin{equation*}
G(t)=a^{6} \sum_{\vec{x}}\left(a m_{q}\right)^{2}\langle 0| j_{5}(\vec{x}, t) j_{5}(0,0)|0\rangle . \tag{2.1}
\end{equation*}
$$

Then the time moments are

$$
\begin{equation*}
G_{n}=\sum_{t}\left(\frac{t}{a}\right)^{n} G(t) \tag{2.2}
\end{equation*}
$$

(see e.g. [1] []). To help reducing the errors we divide each moment by the tree level value, $G_{n}^{(0)}$, and define reduced moments $R_{n}$ as

$$
\begin{equation*}
R_{4}^{\text {latt }}=\frac{G_{4}}{G_{4}^{(0)}}, \quad \text { and } \quad R_{n}^{\text {latt }}=\left(\frac{G_{n}}{G_{n}^{(0)}}\right)^{\frac{1}{n-4}} \text { for } \quad n \geq 6 \tag{2.3}
\end{equation*}
$$

In the continuum the reduced moments are

$$
\begin{equation*}
R_{4}^{\text {cont }}=\frac{g_{4}}{g_{4}^{(0)}}, \quad \text { and } \quad R_{n}^{\text {cont }}=\frac{m_{\eta_{h}}}{2 m_{h}(\mu)} \frac{g_{n}}{g_{n}^{(0)}} \quad \text { for } \quad n \geq 6 \tag{2.4}
\end{equation*}
$$

The $g_{n}$ are perturbative series in $\alpha_{s}(\mu)$, known for the heavy-heavy case through $\alpha_{s}^{3}(\mu)$ [3] and for heavy-light through $\alpha_{s}^{2}(\mu)[母]$. The mass $m_{h}$ is the heavy quark mass in the $\overline{\mathrm{MS}}$ scheme at the scale $\mu$. Comparing the lattice and continuum $R_{n}$ allows us to extract the mass ratio $m_{\eta_{h}} /\left(2 m_{h}(\mu)\right)$, and thus the quark mass. The calculation above is for the case with no $Z$ factor. If the lattice current has a $Z$ factor then that can also be extracted.

## 3. Heavy-light JJ correlators

We compare lattice calculations to continuum perturbation theory through $\alpha_{s}^{2}(\mu)$. In this work we have used coarse, fine, superfine and ultrafine MILC lattice configurations. We calculate heavy-light correlators using the HISQ action [ $[5]$ for both quarks with several heavy quark masses from charm up to the $b$ quark mass. Note that $Z=1$ in the HISQ case. Some of the calculated reduced moments $R_{n}$ are shown in Fig. 1 as examples of our results. Comparing heavy-strange, heavy-charm and heavy-heavy correlator reduced moments shows that we can clearly distinguish between these three cases. In the following subsections we address some challenges of the heavylight calculations.


Figure 1: Top figure: Heavy-strange correlator reduced moments $R_{n}$ as a function of heavy-heavy meson mass $M_{\eta_{h}}$ (in GeV ). The other two figures show the heavy-strange, heavy-charm and heavy-heavy reduced moments $R_{4}$ and $R_{10}$ as a function of $M_{\eta_{h}}$. The range is from charm (at about 3 GeV ) to $b$ (about 10 GeV ).


Figure 2: The reduced moments in the free, non-interacting theory depend on the volume.


Figure 3: The ratio of reduced moments calculated on two different coarse lattices (one with $L=20$, other one with $L=28$ ) shows that there is no volume dependence in the interacting case.

### 3.1 Volume dependence

The tree level (free) moments depend on volume - note that this is an artifact of the free case only. This is illustrated in Figures 2 and 3 - the $R_{n}$ depend on volume in the non-interacting theory, but not in the interacting case. Therefore we need to calculate the tree level moments in the infinite volume limit. We do this by calculating the free moments using different volumes, $L^{3}$, and fitting them with

$$
\begin{equation*}
A_{0}+A_{1} \frac{e^{-A_{2} L}}{L} . \tag{3.1}
\end{equation*}
$$

The result in the infinite volume limit is then simply given by the fit parameter $A_{0}$.


Figure 4: Fraction of the tree level $q \bar{q}$ condensate in reduced moment $R_{n}$ as a function of the heavy-heavy meson mass $M_{\eta_{h}}$ (in GeV ).

### 3.2 Quark condensate

The quark condensate appears in the reduced moment $R_{n}$ at tree level as [6]

$$
\begin{equation*}
\frac{4 \pi^{2}}{3} \frac{(n-1)(n-2)(n-3)\left[-\frac{m_{h}}{m_{l}}+\frac{n}{2}\right]}{1+\frac{(n-3) m_{l}}{m_{h}}} \frac{\left\langle m_{l} \psi \bar{\psi}\right\rangle}{m_{h}^{4}} \tag{3.2}
\end{equation*}
$$

The quark condensate is not present in the heavy-heavy case, but it is sizeable in the heavy-light case - the fraction of tree level $q \bar{q}$ condensate in $R_{n}$ can easily be $10-30 \%$ for heavy quark masses masses between $c$ and $b$, as can be seen in Fig. 4. Note that the leading term is $1 / m_{h}^{3}$. This poses a challenge, as the $\alpha_{s}$ corrections to the condensate are not known. The gluon condensate contribution is much smaller and can be safely neglected in the analysis.

## $3.3 m_{l} / m_{h}$ corrections to perturbative series

Perturbation theory with $m_{q}=0$ is not sufficient, as $m_{l}(\mu) / m_{h}(\mu)$ corrections become important for $B_{c}: m_{c}(\mu) / m_{b}(\mu) \approx 0.22$. At small values of the ratio the $m_{l}(\mu) / m_{h}(\mu)$ expansion is good, i.e. it works for $B_{s}$. At large values of the ratio the expansion is not good enough. This is illustrated in Fig. 5. However, we now have the exact coefficients for given ratios $m_{l}(\mu) / m_{h}(\mu)$ for tree level (shown in the plot as bursts) and order $\alpha_{s}$, so this problem can be partly avoided. The exact coefficients are still needed for $\alpha_{s}^{2}$ and higher orders.

### 3.4 Fits

We fit the lattice data $R_{n}^{\text {latt }}, n \geq 6$, with

$$
\begin{align*}
R_{n}^{\mathrm{fit}}= & \left(\frac{m_{\eta_{h}}}{2 m_{h}(\mu)}\right)\left(1+c_{1} \alpha_{s}+c_{2} \alpha_{s}^{2}+c_{3} \alpha_{s}^{3}+c_{4} \alpha_{s}^{4}+c_{5} \alpha_{s}^{5}+c_{6} \alpha_{s}^{6}+q \bar{q} \quad \text { condensate }\right)  \tag{3.3}\\
& \left(1+b_{1}\left(a m_{h}(\mu)\right)^{2}+b_{2}\left(a m_{h}(\mu)\right)^{4}+b_{3}\left(a m_{h}(\mu)\right)^{6}+d_{1} a^{2}+d_{2} a^{4}\right)
\end{align*}
$$



Figure 5: $m_{l}(\mu) / m_{h}(\mu)$ corrections to continuum perturbation theory coefficients. Here $x=m_{l} / m_{h}$. The tree level values of the coefficients have been divided by the tree level value at $m_{l} / m_{h}=0$.
and choose the scale $\mu=m_{h}$. We take the first few coefficients ( $c_{1}$ and $c_{2}$ in the heavy-light case) from continuum perturbation theory, and treat the coefficients for the higher order $\alpha_{s}$ terms as fit parameters. The quark condensate is given in Eq. 3.2 at tree level. We take the $q \bar{q}$ condensate value to be $\left\langle m_{s} s \bar{s}\right\rangle=(0.2 \mathrm{GeV})^{4}$ from the Gell-Mann - Oakes - Renner relation, allowing the $s \bar{s}$ condensate to be 0.7 times the light quark condensate. We also allow for the presence of higher order condensate terms estimating them with powers of the leading condensate. In $B_{c}$ there is no condensate contribution, and we get a good fit using the exact coefficients (order $\alpha_{s}$ ). As the lattice calculations are done at a non-zero lattice spacing $a$, we include $a$-dependent terms in the fit function - even powers of $a$ and $a m_{h}(\mu)$.

To extract the mass ratio $m_{\eta_{h}} /\left(2 m_{h}(\mu)\right)$ we use the lattice simulation data (Eq. 2.3), with $a m_{\eta_{h}} / a m_{h}$ from the lattice simulations, and compare these $R_{n}^{\text {latt }}$ to the continuum perturbation theory result (Eq. 2.4). That is, we find values for $\alpha_{\overline{\mathrm{MS}}}(\mu)$ and $m_{\eta_{h}} /\left(2 m_{h}(\mu)\right)$ that make lattice and continuum results agree for small $n>4$. This can then be combined with experimental results for the $\eta_{b}, \eta_{c}$ meson masses to obtain the quark masses. In the heavy-light case we can use the $\alpha_{\overline{\mathrm{MS}}}(\mu)$ values extracted from the heavy-heavy calculation.

To test the method in the heavy-light case we look at the mass ratio $m_{\eta_{h}} /\left(2 m_{h}(\mu)\right)$ and compare to heavy-heavy results. This is shown in Figure 6. In the heavy-strange case the fits are to one $R_{n}$ at a time, not to all $R_{n}$ simultaneously as in the heavy-heavy case. The mass ratio extracted from the heavy-strange correlator moments is the same as in the heavy-heavy case, as expected, but currently a lot less accurate.

## 4. Conclusions and future

We are extending the use of current-current correlator method, earlier used to study heavyheavy systems, to heavy-light systems. The full analysis of heavy-light data is still in progress, but we can already say that the JJ correlator method works well. The quark condensate sets some


Figure 6: The mass ratio $m_{\eta_{h}} /\left(2 m_{h}(\mu)\right)$.
limitations - we can not use high moments in the $B_{s}$ case. However, in $B_{c}$ there is no condensate contribution. Our aim is to extract $Z$ for NRQCD - there the challenge is to control relativistic corrections.

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# High-Precision $f_{B_{s}}$ and HQET from Relativistic Lattice QCD 

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#### Abstract

We present a new determination of the $B_{s}$ leptonic decay constant from lattice QCD simulations that use gluon configurations from MILC and a highly improved discretization of the relativistic quark action for both valence quarks. Our result, $f_{B_{s}}=0.225(4) \mathrm{GeV}$, is almost three times more accurate than previous determinations. We analyze the dependence of the decay constant on the heavy quark's mass and obtain the first empirical evidence for the leading $1 / \sqrt{m_{h}}$ dependence predicted by Heavy Quark Effective Theory (HQET). As a check, we use our analysis technique to calculate the $m_{B_{s}}-m_{\eta_{b}} / 2$ mass difference. Our result agrees with experiment to within errors of 11 MeV (better than $2 \%$ ). We discuss how to extend our analysis to other quantities in $B_{s}$ and $B$ physics, making $2 \%$-precision possible for the first time.


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Lattice simulations of QCD have become essential for high-precision experimental studies of $B$-meson decays - studies that test our understanding and the limitations of the standard model of weak, electromagnetic and strong interactions, and also determine fundamental parameters, like the CKM matrix, in that model. Accurate theoretical calculations of QCD contributions to meson masses, decay constants, mixing amplitudes, and semileptonic form factors are critical for this program, and lattice simulation is the main tool for providing these calculations. A major complication for the lattice simulations has been the large mass of the $b$ quark, which has necessitated the use of non-relativistic effective field theories like NRQCD to describe $b$ dynamics in the simulations. The need for effective field theories has made it difficult to achieve better than 5-10\% precision for many important quantities.

Recently we overcame the analogous problem for $c$ quarks by introducing a highly improved discretization of the relativistic quark action that gives accurate results even on quite coarse lattices: the Highly Improved Staggered-Quark (HISQ) discretization [1]. With this formalism, $c$ quarks are analyzed in the same way as $u$, $d$, and $s$ quarks, which greatly reduces the uncertainties in QCD simulations of $D$ physics [2-7]. More recently we showed that the HISQ action can be pushed to much higher masses - indeed, very close to the $b$ mass - using new lattices, from the MILC collaboration, with the smallest lattice spacing available today ( $a=0.044 \mathrm{fm}$ ). This allowed us to extract a value for the $b$ 's $\overline{\mathrm{MS}}$ mass that was accurate to better than $1 \%$. Here we extend that work in a new analysis of the $B_{s}$ meson's leptonic decay constant $f_{B s}$, which produces the most accurate theoretical value to date.

We also compute the mass difference $m_{B_{s}}-m_{\eta_{b}} / 2$, as
an additional test of our analysis method. This difference is particularly sensitive to QCD dynamics because the leading (and uninteresting) dependence on the heavy quark's mass mostly cancels in the difference.

It would be quite expensive to extend our new analysis directly to $B$-meson quantities, because of the added costs associated with very light valence and sea quarks. This is unnecessary, however, because heavy-quark effective field theories like NRQCD already give accurate results for ratios of $B_{s}$ to $B$ quantities, like $f_{B_{s}} / f_{B}$. This is because the largest systematic errors from these effective theories, due to operator matching, cancel in such ratios. The ratio of the decay constants, for example, is known to $\pm 2 \%$ from effective field theories 8]. So the combination of accurate $B_{s}$ quantities from HISQ simulations, as discussed in this paper, with $B_{s} / B$ ratios from NRQCD or other effective field theories provides a potent new approach to high-precision $b$ physics generally. Note that no operator matching is required in our relativistic analysis of $f_{B_{s}}$ because of the exact chiral symmetry of the HISQ formalism in the massless limit.

In our simulations for this paper, we computed decay constants and masses for non-physical $H_{s}$ mesons composed of an $s$ quark, and heavy quarks $h$ with various masses $m_{h}$ ranging from below the $c$ mass to just below the $b$ mass. This data allows us to extrapolate to the $b$ mass, where $m_{H_{s}}=m_{B_{s}}$. We repeated our analysis for five different lattice spacings, allowing us also to extrapolate our results to zero lattice spacing.

The gluon configuration sets we used are from the MILC collaboration [9] and are described in Table [I. Our simulation results for the decay constants and meson masses, for various values of the $h$ mass, are presented in Table [II. We also give results for the mass of the pseudoscalar $h \bar{h}$ meson, $m_{\eta_{h}}$, and for the mass of the $\eta_{s}$


FIG. 1. The leptonic decay constant $f_{H_{s}}$ for pseudoscalar $h \bar{s}$ mesons $H_{s}$, plotted on the left versus the $H_{s}$ mass as the $h$ quark's mass is varied. The solid line and gray band show our best-fit estimates for the decay constants extrapolated to zero lattice spacing. Best-fit results (dashed lines) and simulation data are also shown for five different lattice spacings, with results for smaller lattice spacings extending to higher masses (since we restrict $a m_{h}<1$ ). The simulation data points have been corrected for small mistunings of the $s$ quark's mass. On the right the same simulation data and fits are plotted for $\sqrt{m_{H_{s}}} f_{H_{s}}$ versus $1 / m_{H_{s}}$.

TABLE I. Parameter sets used to generate the 3-flavor gluon configurations analyzed in this paper. The lattice spacing is specified in terms of the static-quark potential parameter $r_{1}=0.3133(23) \mathrm{fm}$ 10]; values for $r_{1} / a$ are from [9]. The bare quark masses are for the ASQTAD formalism and $u_{0}$ is the fourth root of the plaquette. The spatial $(L)$ and temporal $(T)$ lengths of the lattices are also listed, as are the number of gluon configurations ( $N_{\mathrm{cf}}$ ) and the number of time sources ( $N_{\text {ts }}$ ) per configuration used in each case.

| Set | $r_{1} / a$ | $a u_{0} m_{0 u / d}$ | $a u_{0} m_{0 s}$ | $u_{0}$ | $L / a$ | $T / a$ | $N_{\text {cf }} \times N_{\text {ts }}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | $2.152(5)$ | 0.0097 | 0.0484 | 0.860 | 16 | 48 | $631 \times 2$ |
| 2 | $2.618(3)$ | 0.01 | 0.05 | 0.868 | 20 | 64 | $595 \times 2$ |
| 3 | $3.699(3)$ | 0.0062 | 0.031 | 0.878 | 28 | 96 | $566 \times 4$ |
| 4 | $5.296(7)$ | 0.0036 | 0.018 | 0.888 | 48 | 144 | $201 \times 2$ |
| 5 | $7.115(20)$ | 0.0028 | 0.014 | 0.895 | 64 | 192 | $208 \times 2$ |

meson. The $\eta_{s}$ is an unphysical pseudoscalar $s \bar{s}$ meson whose valence quarks are not allowed to annihilate; we use its mass to tune the bare mass of the $s$ quark: simulations show that its mass is $m_{\eta_{s}, \text { phys }}=0.6858(40) \mathrm{GeV}$ when the $s$ mass is correctly tuned [10].

We expect some statistical correlation between results from the same configuration set but with different $h$ quark masses. We have not measured these, but we have verified that our results are insensitive (at the level of $\pm \sigma / 4$ ) to such correlations. We introduce a $50 \%$ correlation for our fits, which increases our final error estimates slightly.

Our strategy for extracting $f_{B_{s}}$ is first to fit our simu-

TABLE II. Simulation results for each of the five configuration sets (Table (I) and several values of the heavy-quark's mass $m_{h}$. The $s$-quark's mass $m_{s}$ is tuned to be close to its physical value. Results are given for: the leptonic decay constant $f_{H_{s}}$ and mass $m_{H_{s}}$ of the pseudoscalar $h \bar{s}$ meson, and masses of the pseudoscalar $h \bar{h}$ and $s \bar{s}$ mesons, $m_{\eta_{h}}$ and $m_{\eta_{s}}$ respectively.

|  | $a m_{s}$ | $a M_{\eta_{s}}$ | $a m_{h}$ | $a M_{H_{s}}$ | $a f_{H_{s}}$ | $a m_{\eta_{h}}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 0.061 | $0.5049(4)$ | 0.66 | $1.3108(6)$ | $0.1913(7)$ | $1.9202(2)$ |
|  | 0.061 | $0.5049(4)$ | 0.81 | $1.4665(8)$ | $0.197(1)$ | $2.1938(2)$ |
| 2 | 0.0492 | $0.4144(2)$ | 0.44 | $0.9850(4)$ | $0.1500(5)$ | $1.4240(1)$ |
|  | 0.0492 | $0.4144(2)$ | 0.63 | $1.2007(5)$ | $0.1559(7)$ | $1.8085(1)$ |
|  | 0.0492 | $0.4144(2)$ | 0.85 | $1.4289(8)$ | $0.161(1)$ | $2.2193(1)$ |
| 3 | 0.0337 | $0.2941(1)$ | 0.3 | $0.7085(2)$ | $0.1054(2)$ | $1.03141(8)$ |
|  | 0.0337 | $0.2941(1)$ | 0.413 | $0.8472(2)$ | $0.1084(2)$ | $1.28057(7)$ |
|  | 0.0337 | $0.2941(1)$ | 0.7 | $1.1660(4)$ | $0.1112(5)$ | $1.86536(5)$ |
|  | 0.0337 | $0.2941(1)$ | 0.85 | $1.3190(5)$ | $0.1123(6)$ | $2.14981(5)$ |
| 4 | 0.0228 | $0.2062(2)$ | 0.273 | $0.5935(2)$ | $0.0750(3)$ | $0.8994(1)$ |
|  | 0.0228 | $0.2062(2)$ | 0.564 | $0.9313(5)$ | $0.0754(6)$ | $1.52542(6)$ |
|  | 0.0228 | $0.2062(2)$ | 0.705 | $1.0811(8)$ | $0.0747(8)$ | $1.80845(6)$ |
|  | 0.0228 | $0.2062(2)$ | 0.85 | $1.228(1)$ | $0.074(1)$ | $2.08753(6)$ |
| 5 | 0.0165 | $0.1548(1)$ | 0.195 | $0.4427(3)$ | $0.0555(3)$ | $0.67113(6)$ |
|  | 0.0165 | $0.1548(1)$ | 0.5 | $0.8038(8)$ | $0.055(1)$ | $1.34477(8)$ |
|  | 0.0165 | $0.1548(1)$ | 0.7 | $1.017(1)$ | $0.053(2)$ | $1.75189(7)$ |
|  | 0.0165 | $0.1548(1)$ | 0.85 | $1.168(2)$ | $0.052(2)$ | $2.04296(7)$ |

lation results for $f_{H_{s}}$ to the HQET-inspired formula 11]

$$
\begin{align*}
& f_{H_{s}}\left(a, m_{H_{s}}, m_{\eta_{s}}\right)= \\
& \quad\left(m_{H_{s}}\right)^{b}\left(\frac{\alpha_{V}\left(m_{H_{s}}\right)}{\alpha_{V}\left(m_{D_{s}}\right)}\right)^{-2 / \beta_{0}} \sum_{i=0}^{N_{m}-1} C_{i}(a)\left(\frac{1}{m_{H_{s}}}\right)^{i} \\
& \quad+c_{s}\left(m_{\eta_{s}}^{2}-m_{\eta_{s}, \text { phys }}^{2}\right) \tag{1}
\end{align*}
$$

where $\beta_{0}=11-2 n_{f} / 3=9$ in our simulations 12], $\alpha_{V}$ is
the QCD coupling in the $V$ scheme [5, 13], and constant $b=-0.5$ from HQET. Here we use $m_{H_{s}}$ as a proxy for the $h$-quark mass since its value for $b$ quarks is known from experiment. The last term in Eq. (11) corrects for tuning errors in the $s$-quark mass; we determined that $c_{s}=0.06(1)$ by repeating our calculations with slightly different $s$ masses [14]. We parameterize

$$
\begin{equation*}
C_{i}(a)=\sum_{j, k, l=0}^{N_{a}-1} c_{i j k l}\left(\frac{a m_{h}}{\pi}\right)^{2 j}\left(\frac{a m_{s}}{\pi}\right)^{2 k}\left(\frac{a \Lambda_{\mathrm{QCD}}}{\pi}\right)^{2 l} \tag{2}
\end{equation*}
$$

with $N_{m}=N_{a}=4$. This expansion is in powers of quark masses and the QCD scale parameter $\Lambda_{\mathrm{QCD}} \approx 0.5 \mathrm{GeV}$ divided by the ultraviolet cutoff for the lattice theory: $\Lambda_{\mathrm{UV}} \approx \pi / a$. The fit parameters are the coefficients $c_{i j k l}$ for each of which we use a prior of $0 \pm 1.5$, which is conservative 15].

Our data for five different lattice spacings and a wide range of masses $m_{H_{s}}$ are presented with our fit results in Fig 1. The reach in $m_{H_{s}}$ grows as the lattice spacing decreases (since we restrict $a m_{h}<1$ ), and deviations from the continuum curve get smaller. The fit is excellent, with a $\chi^{2}$ per degree of freedom of 0.36 while fitting all 17 measurements. The small $\chi^{2}$ results from our conservative priors (we get excellent fits and smaller errors with priors that are half the width).

Having determined the parameters in Eq. (11), the second step in our analysis is to set $M_{H_{s}}=M_{B_{s}}, a=0$, and $m_{\eta_{s}}=m_{\eta_{s} \text {, phys }}$ in that formula to obtain our final value for $f_{B_{s}}$,

$$
\begin{equation*}
f_{B_{s}}=0.225(4) \mathrm{GeV} \tag{3}
\end{equation*}
$$

which agrees well with the previous best NRQCD result of $0.231(15) \mathrm{GeV}$ [16] but is almost four times more accurate. Our result also agrees with the recent result of $0.232(10) \mathrm{GeV}$ from the ETM collaboration, although that analysis includes only two of the three light quarks in the quark sea [17].

The error budget for our result is given in Table III] and shows that the dominant errors come from statistical uncertainties in the simulations, the $m_{H_{s}} \rightarrow m_{B_{s}}$ extrapolation, the $a^{2} \rightarrow 0$ extrapolation, and uncertainties in the scale-setting parameter $r_{1}$. Our analysis of $f_{D_{s}}$ in [6] indicates that finite volume errors, errors due to mistuned sea-quark masses, errors from the lack of electromagnetic corrections, and errors due to lack of $c$ quarks in the sea are all significantly less than $1 \%$, and so negligible compared with our other uncertainties. Our final result is also insensitive to the detailed form of the fit function; for example, doubling the number of terms has negligible effect $(0.03 \sigma)$ on the errors and value.

We have also included in Fig. 1 (right) a plot of $\sqrt{m_{H_{s}}} f_{H_{s}}$ for different values of $m_{H_{s}}$. This shows that there are large non-leading terms in $f_{H_{s}}$, beyond the leading $1 / \sqrt{m_{H_{s}}}$ behavior predicted by HQET. Our simulation nevertheless provides evidence for the leading

TABLE III. Dominant sources of uncertainty in our determinations of the $B_{s}$ decay constant and the $B_{s}-\eta_{b}$ mass difference. Contributions are shown from the extrapolations in $m_{H_{s}}, a^{2}$ and $m_{s}$, as well as statistical errors in the simulation data and errors associated with the scale-setting parameter $r_{1}$. Other errors are negligible.

|  | $f_{B_{s}}$ | $m_{B_{s}}-m_{\eta_{b}} / 2$ |
| ---: | :---: | :---: |
| Monte Carlo statistics | $1.30 \%$ | $1.49 \%$ |
| $m_{H_{s}} \rightarrow m_{B_{s}}$ extrapolation | 0.81 | 0.05 |
| $r_{1}$ uncertainty | 0.74 | 0.33 |
| $a^{2} \rightarrow 0$ extrapolation | 0.63 | 0.76 |
| $m_{\eta_{s}} \rightarrow m_{\eta_{s}, \text { phys }}$ extrapolation | 0.13 | 0.18 |
| $r_{1} / a$ uncertainties | 0.12 | 0.17 |
| Total | $1.82 \%$ | $1.73 \%$ |

term. Treating exponent $b$ in Eq. (11) as a fit parameter, rather than setting it equal to -0.5 , we find a best-fit value of $b=-0.51(13)$, in excellent agreement with the HQET prediction. This is the first empirical evidence for this behavior.

Our analysis also yields a value for $f_{D_{s}}$, which agrees with [6]. It is also clear from Fig. [1 (left) that $f_{H_{s}}$ peaks between $f_{D_{s}}$ and $f_{B_{s}}$, and that $f_{B_{s}}$ is smaller - we find:

$$
\begin{equation*}
f_{B_{s}} / f_{D_{s}}=0.906(14) \tag{4}
\end{equation*}
$$

HQET suggests a ratio less than one, but previous lattice QCD results have been ambiguous about this point.

To check our $f_{B s}$ analysis technique, we adapted the same technique to compute the mass difference [18]

$$
\begin{equation*}
\Delta \equiv m_{H_{s}}-m_{\eta_{h}} / 2 \tag{5}
\end{equation*}
$$

using, as inputs, the masses $m_{\eta_{h}}$ computed in our simulations for pseudoscalar $h \bar{h}$ mesons made of our heavy quark. Our values for $\Delta$ come from the results in Table II. We fit them to

$$
\begin{align*}
& \Delta\left(a, m_{H_{s}}, m_{\eta_{s}}\right)= \\
& \quad m_{H_{s}} \sum_{i=0}^{N_{m}-1} D_{i}(a)\left(\frac{1}{m_{H_{s}}}\right)^{i}+d_{s}\left(m_{\eta_{s}}^{2}-m_{\eta_{s}, \mathrm{phys}}^{2}\right) \tag{6}
\end{align*}
$$

where our simulations indicate that $d_{s}=0.18$ (1) [19], and $D_{i}(a)$ has an expansion similar to that for $C_{i}(a)$ (Eq. (2)), with the same priors.

We show the best fit to our simulation data in Fig. 2. Again, the fit is excellent, which a $\chi^{2}$ per degree of freedom of 0.13 while fitting all 17 measurements. Extrapolating to the $b$ mass, we obtain our best fit value for the mass splitting,

$$
\begin{equation*}
m_{B_{s}}-m_{\eta_{b}} / 2=0.658(11) \mathrm{GeV} \tag{7}
\end{equation*}
$$

which agrees well with experiment: experiment gives $0.671(2) \mathrm{GeV}$ which becomes $0.666(4)$ after removing


FIG. 2. The $H_{s}-\eta_{h} / 2$ mass difference plotted versus $m_{H_{s}}$ as the $h$ quark's mass is varied. The solid line and gray band show our best-fit estimates for the mass differences extrapolated to zero lattice spacing. Best-fit results (dashed lines) and simulation data are also shown for five different lattice spacings, with results for smaller lattice spacings extending to larger masses (since we require $a m_{h}<1$ ). The simulation data points have been corrected for small mistunings in the $s$ quark's mass. Data points (in black) at $m_{D_{s}}$ and $m_{B_{s}}$ are the experimental values after correcting for small effects from electromagnetism, $\eta_{b}$ annihilation, and $c$ quarks in the sea, none of which are included in the simulation.
corrections from electromagnetism, $\eta_{b}$ annihilation, and $c$ quarks in the sea (not included in our simulations) [18, 20]. Our fit also gives a value for $m_{D_{s}}-m_{\eta_{c}} / 2$; it also agrees well with experiment [6].

In this paper, we have shown how to use a highly improved discretization of the relativistic quark action to make accurate calculations for mesons containing $b$ quarks. Our result for the $B_{s}$ decay constant, $f_{B_{s}}=$ $0.225(4) \mathrm{GeV}$, agrees with other determinations from lattice QCD but is almost three times more accurate than the most precise previous result. The reliability of our extrapolations is underscored both by our previous determination of the $b$-quark's $\overline{\mathrm{MS}}$ mass, which agrees with other determinations to within errors of less than $\pm 1 \%$, and by our calculation here of the $m_{B_{s}}-m_{\eta_{b}} / 2$ mass difference, which agrees with experiment to within errors of $\pm 11 \mathrm{MeV}$ or less than $2 \%$. Our analysis of the decay constant gives the most extensive information to date on the heavy-quark mass dependence of the decay constant, and provides the first empirical evidence for the leading $1 / \sqrt{m_{h}}$ dependence predicted by HQET. Further results on the $B_{c}$ mesons, and the decay constant $f_{\eta_{h}}$ will be presented elsewhere 21].

Our analysis has important implications for future lattice simulations of $B$ physics. Other $B_{s}$ quantities, like semileptonic form factors, can be analyzed in the same way, bringing few-percent precision within reach. Similar precision for $B$ quantities is possible by combining $B_{s}$
calculations like these with precise calculations of $B_{s} / B$ ratios using (very efficient) non-relativistic effective field theories for $b$-quark dynamics.

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# Fast Fits for Lattice QCD Correlators 

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#### Abstract

We illustrate a technique for fitting lattice QCD correlators to sums of exponentials that is significantly faster than traditional fitting methods - 10-40 times faster for the realistic examples we present. Our examples are drawn from a recent analysis of the $\Upsilon$ spectrum, and another recent analysis of the $D \rightarrow \pi$ semileptonic form factor. For single correlators, we show how to simplify traditional effective-mass analyses.


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Most physics results in lattice QCD come from fits of lattice correlators to sums of exponentials. For example, we study a particular hadron by computing Monte Carlo simulation estimates $G_{a b}^{\mathrm{MC}}(t)$ of hadronic correlators,

$$
\begin{equation*}
\sum_{\mathbf{x}}\langle 0| \Gamma_{b}(\mathbf{x}, t) \Gamma_{a}(0,0)|0\rangle, \tag{1}
\end{equation*}
$$

with different sources $\Gamma_{a}$ and sinks $\Gamma_{b}$ that create and destroy the hadron. The sum over all spatial sites $\mathbf{x}$ restricts the hadrons to states with zero total three-momentum. Such a correlator can be decomposed into contributions from energy eigenstates $\left|E_{j}\right\rangle$ in QCD [1]:

$$
\begin{equation*}
G_{a b}(t ; N)=\sum_{j=1}^{N} a_{j} b_{j} \exp \left(-E_{j} t\right) \tag{2}
\end{equation*}
$$

where $E_{j}$ is the energy, with $E_{j} \geq E_{j-1}$, and the amplitudes are matrix elements, with

$$
\begin{align*}
a_{j}^{*} & =\langle 0| \Gamma_{a}(0,0)\left|E_{j}\right\rangle \\
b_{j} & =\langle 0| \Gamma_{b}(0,0)\left|E_{j}\right\rangle \tag{3}
\end{align*}
$$

The physics is in the energies and the matrix elements, and these are determined by fitting fomula (2) to the Monte Carlo data $G_{a b}^{\mathrm{MC}}(t)$ for a variety of sources and sinks.

In principle, the number of terms $N$ in Eq. (2) is infinite, but, in practice, we need only retain a finite number of terms because the exponentials suppress high-energy states. The number needed depends upon the precision of the simulation data $G_{a b}^{\mathrm{MC}}$, but it is not uncommon to require $N=10$ or more terms for good fits to accurate data. The fitting process becomes both cumbersome and time consuming if many correlators must be fit simultaneously while using such large $N \mathrm{~s}$. In this paper we introduce a method that can dramatically simplify and accelerate such fits.

The key to this new approach lies in how priors are introduced. Two types of input data are required for these fits. The

[^298]first is simulation data for the correlators, consisting of Monte Carlo averages $\bar{G}$ for each $a, b$ and $t$, and a covariance matrix $\sigma^{2}$ that specifies both the statistical uncertainties in each average and the correlations between them:
\[

$$
\begin{equation*}
G_{a b}^{\mathrm{MC}}(t) \leftrightarrow\left\{\bar{G}_{a b}(t), \sigma_{a b, a^{\prime} b^{\prime}}^{2}\left(t, t^{\prime}\right)\right\} \tag{4}
\end{equation*}
$$

\]

This data contributes

$$
\begin{gather*}
\chi_{\mathrm{MC}}^{2}\left(a_{j}, b_{j}, E_{j}\right)=\sum_{t, a, b t^{\prime}, a^{\prime}, b^{\prime}} \sum_{a b}\left(G_{a b}(t ; N)-\bar{G}_{a b}(t)\right) \\
\sigma_{a b, a^{\prime} b^{\prime}}^{-2}\left(t, t^{\prime}\right)\left(G_{a^{\prime} b^{\prime}}\left(t^{\prime} ; N\right)-\bar{G}_{a^{\prime} b^{\prime}}\left(t^{\prime}\right)\right) \tag{5}
\end{gather*}
$$

to the $\chi^{2}$ function that is minimized by varying parameters $a_{j}$, $b_{j}$, and $E_{j}$ in a conventional fit.

The second type of input data consists of Bayesian priors for each fit parameter. Complicated multi-correlator, multiparameter fits are impossible without a priori estimates for each fit parameter [2]:

$$
\begin{gather*}
a_{j}^{\mathrm{pr}} \equiv \bar{a}_{j} \pm \sigma_{a_{j}}, \\
b_{j}^{\mathrm{pr}} \equiv \bar{b}_{j} \pm \sigma_{b_{j}}, \\
E_{j}^{\mathrm{pr}} \equiv \bar{E}_{j} \pm \sigma_{E_{j}} . \tag{6}
\end{gather*}
$$

This information is included in a conventional fit by adding extra terms to $\chi^{2}\left(a_{j}, b_{j}, E_{j}\right): \chi^{2}=\chi_{\mathrm{MC}}^{2}+\chi_{\mathrm{pr}}^{2}$ where

$$
\begin{align*}
& \chi_{\mathrm{pr}}^{2}\left(a_{j}, b_{j}, E_{j}\right)= \\
& \quad \sum_{j=1}^{N}\left\{\frac{\left(a_{j}-\bar{a}_{j}\right)^{2}}{\sigma_{a_{j}}^{2}}+\frac{\left(b_{j}-\bar{b}_{j}\right)^{2}}{\sigma_{b_{j}}^{2}}+\frac{\left(E_{j}-\bar{E}_{j}\right)^{2}}{\sigma_{E_{j}}^{2}}\right\} . \tag{7}
\end{align*}
$$

The priors can also be combined to give a priori estimates for the correlators,

$$
\begin{equation*}
G_{a b}^{\mathrm{pr}}(t ; N) \equiv \sum_{j=1}^{N} a_{j}^{\mathrm{pr}} b_{j}^{\mathrm{pr}} \exp \left(-E_{j}^{\mathrm{pr}} t\right) \tag{8}
\end{equation*}
$$

where the means and covariance matrix for $G_{a b}^{\mathrm{pr}}(t)$ are computed, using standard error propagation, from the means and covariance matrix of the priors (Eq. (6)).

The cost of a traditional analysis goes up rapidly with the number of parameters needed to obtain a good fit. In practice, however, we are rarely interested in parameters from the large$j$ terms in fit function (2), even when these terms are needed for a good fit. Rather than including them in the fit, we can incorporate the large- $j$ terms into the Monte Carlo data before fitting. To do this, we use the priors to generate an a priori estimate for these terms, and then subtract that estimate from the Monte Carlo data. This effectively removes the large- $j$ terms from the data. Finally we fit the modified data with a simpler formula that includes only small- $j$ terms.

More explicitly, we can remove terms having $n<j \leq N$ by replacing $G_{a b}^{\mathrm{MC}}(t)$ with (first definition)

$$
\begin{equation*}
\tilde{G}_{a b}^{\mathrm{MC}}(t ; n) \equiv G_{a b}^{\mathrm{MC}}(t)-\Delta G_{a b}^{\mathrm{pr}}(t ; n) \tag{9}
\end{equation*}
$$

where

$$
\begin{align*}
\Delta G_{a b}^{\mathrm{pr}}(t ; n) & \equiv G_{a b}^{\mathrm{pr}}(t ; N)-G_{a b}^{\mathrm{pr}}(t ; n) \\
& =\sum_{j=n+1}^{N} a_{j}^{\mathrm{pr}} b_{j}^{\mathrm{pr}} \exp \left(-E_{j}^{\mathrm{pr}} t\right) \tag{10}
\end{align*}
$$

is the $j>n$ part of the fit function. Having removed the $j>n$ terms, we can fit $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$ with the simpler fit function, $G_{a b}(t ; n)$, rather than $G_{a b}(t ; N)$.

Here we assume that $N$ is sufficiently large that $\Delta G_{a b}^{\mathrm{pr}}(t ; n)$ and therefore $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$ are independent of $N$ to within their statistical errors. The covariance matrix for $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$ is obtained by adding the covariance matrices of $G_{a b}^{\mathrm{MC}}(t)$ and $\Delta G_{a b}^{\mathrm{pr}}(t ; n)$ (that is, adding the errors in quadrature) [4].

Removing high- $j$ terms from both the fit function and the fit data replaces the original fitting problem - fit an $N$-term function $G_{a b}(t ; N)$ to $G_{a b}^{\mathrm{MC}}(t)$ - by a simpler problem that can have far fewer fit parameters: fit an $n$-term function $G_{a b}(t ; n)$ to $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$, where $n<N$. Remarkably, as we showed in [3], these two problems are equivalent for high statistics data even when $n$ is quite small: that is, fit results (means and standard deviations) for the low- $j$ parameters are the same in both cases. In the second case, the $j>n$ terms have been "marginalized," or, in effect, integrated out of the Bayesian probability distribution, but in a way that does not affect the analysis of the $j \leq n$ terms. When $n \ll N$, the fit parameters that remain are many fewer than what would be required in a standard fit, and fitting is much faster.

In this paper we use a variation of this marginalization procedure which we find to be more robust when fitting correlators that fall exponentially quickly with increasing $t$. In this variation the modified correlators are given by (second definition)

$$
\begin{equation*}
\tilde{G}_{a b}^{\mathrm{MC}}(t ; n) \equiv G_{a b}^{\mathrm{MC}}(t) \frac{G_{a b}^{\mathrm{pr}}(t ; n)}{G_{a b}^{\mathrm{pr}}(t ; N)} \tag{11}
\end{equation*}
$$

which is analogous to the first definition (Eq. (9)) but applied to the logarithm of the correlator rather than the correlator itself. Again, terms with $j>n$ have been removed, and therefore the modified correlator data can be fit with the simpler fit function, $G_{a b}(t ; n)$.


FIG. 1. Fit $\chi^{2}$ per degree of freedom for sequential fits of $25 \Upsilon$ correlators with $n=1,2,3 \ldots$ terms in fit function (2). Results are plotted versus the cumulative time required for fitting, and are for fits of: a) the unmodified simulation data $G_{a b}^{\mathrm{MC}}(t)$ (red circles and dotted line); and b) the modified simulation data $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$ (Eq. (11)) (blue circles and dashed line). The region of good fits is indicated by the gray band.

We now illustrate our new method by applying it to QCD simulation data from two recent analyses. For each analysis, we fit a function, like $G_{a b}(t ; n)$, with $n$ terms both to untouched simulation data $G_{a b}^{\mathrm{MC}}(t)$, and to modified simulation data $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$, from which $j>n$ terms have been removed using Eq. (11). We vary $n$, doing sequential fits with $n=1,2,3 \ldots$, where the best-fit parameter values from one fit are used as starting values for the next fit. Sequential fitting with increasing $n$ is a standard approach to complicated multiparameter correlator fits; $n$ is increased until the fit's $\chi^{2}$ stops changing, at which point enough terms have been include to reflect accurately the uncertainties introduced by large- $j$ terms. Here we examine the best-fit parameters for each $n$ to investigate the rate at which correct results emerge from this process. This allows a detailed comparison of our two fitting strategies.

The first data set is a collection of 25 correlators for the $\Upsilon(1 S)$ meson and its radial excitations $(\Upsilon(2 S), \Upsilon(3 S)$, etc.) [5]. These correlators were made using five different operators for both sources and sinks. They were fit to formula (2) with priors (in lattice units):

$$
\begin{align*}
\log \left(E_{1}\right) & =\log (0.3 \pm 0.1)=-1.2 \pm 0.3 \\
\log \left(E_{j+1}-E_{j}\right) & =\log (0.25 \pm 0.125)=-1.4 \pm 0.5 \\
a_{j} & =0.1 \pm 1.0 \tag{12}
\end{align*}
$$

except for a local source for which the priors were $\log \left(a_{j}\right)=$ $\log (0.1 \pm 0.2)=-2.3 \pm 2$ (local source). These are broad priors - more than 100 times broader than the final errors for the quantities we examine below. We set $N=20$ when defining $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$ (Eq. (11)); this is roughly twice the size it needs to be, but it costs little to make $N$ large. In general $N$ should be chosen so that terms with $j>N$ are negligible compared with statistical errors.

In Fig. 11 we plot the $\chi^{2}$ per degree of freedom for each method versus the time required to get to that value [6]. As expected, the new algorithm reaches a reasonable $\chi^{2}$ with just a few terms $(n=2-3)$, in 20-30 seconds; the traditional al-


FIG. 2. Best-fit results from sequential fits of $25 \Upsilon$ correlators with $n=1,2,3 \ldots$ terms in fit function (2). Results are plotted versus the cumulative time required for fitting, and are for fits of: a) the unmodified simulation data $G_{a b}^{\mathrm{MC}}(t)$ (red circles and dotted line); and b) the modified simulation data $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$ (Eq. (111) (blue circles and dashed line). Results are given for mass splittings between different vector $S$-states, and for the wave functions at the origin for the lowest two states. All results are in lattice units. The gray bands show the best-fit result from the modified data after convergence.
gorithm requires $n=10-11$ to obtain a good $\chi^{2}$, and 600700 seconds. Similar differences are evident if we look at physical quantities extracted from the simulations. In Fig. 2 we show results for the $2 S-1 S$ mass splitting (in lattice units), for the $3 S-1 S$ mass splitting divided by the $2 S-1 S$ splitting, and for the $1 S$ and $2 S$ mesons' (nonrelativistic) wave functions at the origin, which come from fit parameters $a_{j}$ for a local source. In every case the two algorithms agree on the final result, but the new algorithm converges to correct results


FIG. 3. Best-fit results from sequential fits of 13 two-point and threepoint correlators for $D$ and $\pi$ mesons with $n=1,2,3 \ldots$ terms in fit function (2). Results are plotted versus the cumulative time required for fitting, and are for fits of: a) the unmodified simulation data (red circles and dotted line); and b) the modified simulation data (Eq. 11) (blue circles and dashed line). Results are given for the $D$-meson mass $m_{D}$ and decay constant $f_{D}$, and for the $D \rightarrow \pi$ scalar form factor at zero recoil momentum $f_{0}(0,0,0)$. All results are in lattice units. The gray bands show the best-fit result from the modified data after convergence.

## 10-40 times faster.

Our second example is from a recent analysis of the $D \rightarrow$ $\pi$ semileptonic form factor [7]. To extract the form factor at four different momenta, this analysis uses a simultaneous fit of 13 two-point and three-point correlators: a) a $D$-meson correlator with a pseudoscalar local source and sink; b) four $\pi$-meson correlators, one for each pion momentum of interest, again with local pseudoscalar sources and sinks; and c) two three-point correlators $D \rightarrow J_{\text {scalar }} \rightarrow \pi$ for each of the four pion momenta. The fit functions are more complicated for this case. For example, the $D$-meson correlator is fit by a function:

$$
\begin{equation*}
G_{D}(t ; n)=\sum_{j=1}^{n} a_{j} f\left(E_{j}, t\right)-(-1)^{t} a_{j}^{o} f\left(E_{j}^{o}, t\right) \tag{13}
\end{equation*}
$$

where $f\left(E_{j}, t\right) \equiv \exp \left(-E_{j} t\right)+\exp \left(-E_{j}(T-t)\right)$ is periodic with period $T=64$, and the second (oscillating) term is due to


FIG. 4. The $D$-meson's effective mass $m_{\text {eff }}(t)$ versus $t$ computed from modified simulation data $\tilde{G}_{D}^{\mathrm{MC}}(t)$ from which every state other than the ground state has been removed (using priors). The (very thin) gray band shows the weighted average of all $m_{\text {eff }}(t) \mathrm{s}$, taking account of correlations. The thickness of the band indicates the uncertainty of the average. Note that the largest $t \mathrm{~s}$ shown here correspond to the middle $t$ range. The error bars grow there because $m_{\text {eff }}(t)$ becomes very sensitive to statistical errors in this region (since periodic boundary conditions imply that the derivative of the correlator's nonoscillating part vanishes at the midpoint).
opposite-parity states in the correlator (a feature of staggeredquark formalisms like that used in this analysis). The details for the other correlators, and the priors are given in [7].

Despite the complexity of dealing with both two-point and three-point correlators, this is a simpler fit than the $\Upsilon$ case; but even here we find that marginalizing most of the fit function makes the analysis about 30 times faster. We show results in Fig. 3for the $D$-meson's mass $m_{D}$ and leptonic decay constant $f_{D}$, as well as for the $D \rightarrow \pi$ scalar form factor $f_{0}(0,0,0)$ at zero recoil momentum. All results are in lattice units. Again the two approaches agree on the results but the new approach has correct results even with only a single term $(n=1)$ in the fit functions. For these fits we set $N=10$ when computing the modified data $\tilde{G}_{a b}^{\mathrm{MC}}(t ; n)$ (Eq. (11)), which is twice as large as it needs to be.

Some insight into how marginalization works can be gained by focusing just on the $D$ correlator from this analysis and fitting the modified data,

$$
\begin{equation*}
\tilde{G}_{D}^{\mathrm{MC}}(t) \equiv G_{D}^{\mathrm{MC}}(t) \frac{a_{1}^{\mathrm{pr}} f\left(E_{1}^{\mathrm{pr}}, t\right)}{G_{D}^{\mathrm{pr}}(t ; N)} \tag{14}
\end{equation*}
$$

with only the non-oscillating part of the first term in Eq. (13) - that is, with $a_{1} f\left(E_{1}, t\right)$. This situation is sufficiently simple that fitting is not required. The $D$ mass, for example, can be obtained by averaging the "effective mass,"

$$
\begin{equation*}
m_{\mathrm{eff}}(t) \equiv \operatorname{arccosh}\left(\frac{\tilde{G}_{D}^{\mathrm{MC}}(t+1)+\tilde{G}_{D}^{\mathrm{MC}}(t-1)}{2 \tilde{G}_{D}^{\mathrm{MC}}(t)}\right) \tag{15}
\end{equation*}
$$

over all $t$, taking account of correlations between different $t \mathrm{~s}$.

The effective mass is plotted as a function of $t$ in Fig. 4 It is compared with the weighted average of all $27 m_{\text {eff }}(t) \mathrm{s}$ (gray band), which at $m_{\text {eff }}^{\text {avg }}=1.1584(11)$ agrees well with the best result, 1.1593(7), from full multi-term fits (top panel in Fig. 37.

The first excited state in the $D$ correlator is the oppositeparity contribution, which accounts for the oscillation in $m_{\text {eff }}(t)$. Strong statistical correlations between different points result in an average $m_{\text {eff }}$ whose error is more than 7 times smaller than the best error from an individual $m_{\text {eff }}(t)$. The errors in $m_{\text {eff }}(t)$ when $t \leq 16$ come almost entirely from marginalized terms absorbed into the fit data using Eq. (14); the original Monte Carlo simulation errors are negligible there.

Absent marginalization, contributions from excited states would limit a traditional effective mass analysis of this data to values with $t>16$. With marginalization, all $t \mathrm{~s}$ are used, except for a small number at very small $t$ where the fit function is invalid (because of temporal non-locality in the lattice quark action). Using $28 t \mathrm{~s}$ is possible because we have removed the excited states through Eq. (14). As a result different $m_{\text {eff }}(t) \mathrm{s}$ agree with each other to within their errors: fitting all 27 values in Fig. 4 to a constant gives an excellent fit, with a $\chi^{2}$ per degree of freedom of 0.6 . (The result of the fit is, by definition, the same as the weighted average reported above.)

Our new implementation of effective-mass analyses is simpler and less ambiguous than traditional analyses because we are not limited to large $t \mathrm{~s}$. More importantly our implementation also allows us to quantify the contribution to the uncertainty in the final $m_{\text {eff }}^{\text {avg }}$ due to the excited states: here the priors for non-oscillating terms in Eq. (13) contribute $0.44 \sigma_{m}$, those from oscillating terms contribute $0.07 \sigma_{m}$, and the uncertainties in the Monte Carlo data contribute $0.89 \sigma_{m}$, where $\sigma_{m}$ is the standard deviation of $m_{\mathrm{eff}}^{\text {avg }}$. Such information is essential for assessing the reliability of the final result, as well as for planning improvements to the analysis.

In this paper we have shown how to accelerate multiexponential fits to multiple hadronic correlators by removing contributions due to excited states from both the fit function and the simulation data, before fitting. This technique for marginalizing large parts of the fit function greatly reduces the number of fit parameters needed in the realistic examples presented here, and makes fitting 10-40 times faster. Marginalization also simplifies effective-mass analyses, and generalizes easily to analogous multi-state (generalized eigenvalue) methods.

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[1] Lattice QCD simulations use Euclidean time and so -it is replaced by $-t$ in the exponentials. Also simulations are for finite
volumes in space, and therefore all states, including multi-hadron
states, have discrete energy eigenvalues.
[2] G. P. Lepage, B. Clark, C. T. H. Davies, K. Hornbostel, P. B. Mackenzie, C. Morningstar, H. Trottier, Nucl. Phys. Proc. Suppl. 106, 12-20 (2002). |hep-lat/0110175|. The formula for $\chi_{\mathrm{pr}}^{2}$ generalizes trivially if there are correlations between the priors for different parameters.
[3] For a proof, see the appendix of C. McNeile, C. T. H. Davies, E. Follana, K. Hornbostel, G. P. Lepage, Phys. Rev. D82, 034512 (2010). [arXiv:1004.4285 [hep-lat]].
[4] Again the covariance matrix for $\Delta G_{a b}(t ; n)$ is computed using standard error propagation - for example, $f\left(\bar{x} \pm \sigma_{x}\right)=\bar{f} \pm \sigma_{f}$ with $\bar{f} \approx f(\bar{x})$ and $\sigma_{f}^{2} \approx f^{\prime}(\bar{x})^{2} \sigma_{x}^{2}$. We have compared this linearized analysis with Monte Carlo evaluations of $\Delta G$ (from normal distributions for the priors). We find the Monte Carlo results to be both much more expensive and also less robust for correlators that decay exponentially quickly. Note also that it is essential to retain the off-diagonal elements (correlations) in the covariance matrix for $\Delta G_{a b}(t ; n)$; correlations arise because, for
example, the prior data used for a parameter is the same for all $t$ values.
[5] The simulations used 0.09 fm lattices with $n_{f}=4$ sea quarks (HISQ discretization), and NRQCD dynamics for the $b$ quark. The gluon configurations were provided by the MILC collaboration. For further details see: R. J. Dowdall, et al., [arXiv:1110.6887][hep-lat]].
[6] The absolute computer times quoted here are obviously of little relevance since they depend upon specific details of hardware and software. What is relevant is the comparison between methods.
[7] The simulations used 0.12 fm lattices with $n_{f}=3$ light sea quarks (ASQTAD discretization), and HISQ relativistic dynamics for valence quarks. The gluon configurations were provided by the MILC collaboration. For further details see (set C2): H. Na, C. T. H. Davies, E. Follana, J. Koponen, G. P. Lepage, J. Shigemitsu, arXiv:1109.1501 [hep-lat].

# Heavy meson masses and decay constants from relativistic heavy quarks in full lattice QCD 

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#### Abstract

We determine masses and decay constants of heavy-heavy and heavy-charm pseudoscalar mesons as a function of heavy quark mass using a fully relativistic formalism known as Highly Improved Staggered Quarks for the heavy quark. We are able to cover the region from the charm quark mass to the bottom quark mass using MILC ensembles with lattice spacing values from 0.15 fm down to 0.044 fm . We obtain $f_{B_{c}}=0.427(6) \mathrm{GeV} ; m_{B_{c}}=6.285(10) \mathrm{GeV}$ and $f_{\eta_{b}}=0.667(6)$ GeV. Our value for $f_{\eta_{b}}$ is within a few percent of $f_{\Upsilon}$ confirming that spin effects are surprisingly small for heavyonium decay constants. Our value for $f_{B_{c}}$ is significantly lower than potential model values being used to estimate production rates at the LHC. We discuss the changing physical heavyquark mass dependence of decay constants from heavy-heavy through heavy-charm to heavy-strange mesons. A comparison between the three different systems confirms that the $B_{c}$ system behaves in some ways more like a heavy-light system than a heavy-heavy one. Finally we summarise current results on decay constants of gold-plated mesons.


## I. INTRODUCTION

Lattice QCD calculations offer particular promise for $B$ meson physics where a number of relatively simple weak decay processes give access to elements of the CKM matrix that are important for constraining the unitarity triangle of the Standard Model [1]. The theoretical calculation of the appropriate weak matrix elements must be done with percent accuracy for stringent constraints, making optimal use of the experimental results. This has not yet been achieved, despite the enormous success of lattice QCD over the last five years and its acceptance as a precision tool for QCD physics [2]. Work is ongoing on several different approaches. Here we continue discussion of an alternative method for $B$ meson physics that may offer a faster route to high accuracy for some quantities than other methods currently in use. Following work on accurate $b$ and $c$ quark masses [3] and heavy-strange decay constants [4, we show results for masses and decay constants of $B_{c}$ and $\eta_{b}$ mesons and map out their heavy-quark mass dependence. As well as showing that high accuracy can be achieved, these results provide an interesting comparison of how heavy-charm mesons sit between heavy-heavy and heavy-light.

The calculations use a discretisation of the quark Lagrangian onto the lattice known as the Highly Improved Staggered Quark (HISQ) action 5]. This has the advantages of being numerically very fast along with having small discretisation errors and enough chiral symmetry

[^299](a PCAC relation) that the weak current that causes charged pseudoscalar mesons to decay leptonically is absolutely normalised. This action readily gives $\pi$ and $K$ meson decay constants with errors below $1 \%$ on gluon field configurations that include the full effect of $u, d$ and $s$ quarks in the sea [6, 7]. Results from multiple values of the lattice spacing and multiple sea $u / d$ quark masses allow extrapolation to the real world with physical $u / d$ quark masses at zero lattice spacing.

The HISQ action gives similarly accurate results for mesons containing $c$ quarks [6], significantly improving on previous methods that use a nonrelativistic effective theory such as the Fermilab action [8] or NRQCD [9]. The key advantages are clear: the HISQ action has no errors from missing higher order terms in the effective theory or from the renormalisation of the decay constant [1]. The price to be paid is that of the discretisation errors. These errors are much larger for $c$ quarks than for $u / d$ and $s$, since their size is now set by $m_{c} a$ rather than $\Lambda_{Q C D} a$. They can be well controlled, however, using the HISQ action on gluon configurations with a wide range of lattice spacing values down to 0.045 fm where $m_{c} a=$ 0.2 [10]. Discretisation errors are in fact the only issue for the $D_{s}$ meson, for which particularly accurate results can be obtained. This meson has no valence light quarks and the dependence of both its mass and decay constant on the $u / d$ quark masses is seen to be very small [10], meaning that uncertainties from the chiral extrapolation are not significant.

It is less clear what to do for $b$ quarks because they are so much heavier. To achieve $m_{b} a<1$ we need a lattice spacing, $a<0.04 \mathrm{fm}$. Using NRQCD or the Fermilab formalism we can readily handle $b$ quarks on much coarser lattices, with $a \approx 0.1 \mathrm{fm}$, but must then take a substan-
tial error (currently $4 \%$ for NRQCD [11]) from matching the weak annihilation current to full QCD perturbatively. Work is underway to reduce this error [12]. It should also be emphasised that this matching error is not present in ratios of decay constants, for example $f_{B_{s}} / f_{B}$ which is known to $2 \%$ from NRQCD [11].

Here we show what accuracy is possible using the HISQ action for $b$ quarks. We use quark masses heavier than that of the $c$ quark and map out the heavy quark mass dependence of both masses and decay constants for a variety of different pseudoscalar mesons. By using experience from the $D_{s}[10$ and concentrating on mesons that do not contain valence light quarks we do not have to worry significantly about the extrapolation to the physical $u / d$ quark mass limit. The key issue is that of discretisation errors, as for $f_{D_{s}}$, and we therefore work with the same large range of lattice spacing values from 0.15 fm to 0.044 fm , so that we can account fully for the $a$ dependence. It is important to separate discretisation effects from physical dependence on the heavy quark mass since we do also have to extrapolate to the physical $b$ mass from the quark masses that we are able to reach on these lattices. We are only able to obtain results directly at close to the physical $b$ mass on the finest, 0.044 fm lattice.

We have already demonstrated how well this method works in determining the decay constant of the $B_{s}$ meson [4], one of the key quantities of interest for CKM studies. Mapping out the $B_{s}$ decay constant as a function of heavy quark mass showed that the decay constant peaks around the $D_{s}$ and then falls slowly. We found that $f_{B_{s}} / f_{D_{s}}=0.906(14)$, the first significant demonstration that this ratio is less than 1.

Here we extend this work to map out results for the decay constants of the $\eta_{b}$ and $B_{c}$ mesons, along with the $B_{c}$ meson mass. The $B_{c}$ meson mass is known experimentally but its leptonic decay rate has not yet been measured and so we provide the first prediction of that in full lattice QCD. The masses and decay constants also reveal information about the nature of these mesons that can provide useful input to model calculations. For example, does the $B_{c}$ meson look more like a heavy-heavy meson or a heavy-light meson? It is important to emphasise that both the results determined at the $b$ quark mass and the dependence on the heavy quark mass (and on any light quark masses) have physical meaning: the former can be tested against experiment but the latter can provide stringent tests of models and comparison between lattice QCD calculations.

The layout of the paper is as follows: section II describes the lattice calculation and then section III gives results for heavy-heavy and heavy-charm mesons in turn. We compare the $B_{c}$ meson mass to experiment and predict its decay constant as well as comparing the behaviour of heavy-charm mesons to that of heavyonium and heavy-strange mesons. Section V gives our conclusions, looking forward to what will be possible for $b$ quark physics on even finer lattices in future.

| Set | $r_{1} / a$ | $a u_{0} m_{l}^{a s q}$ | $a u_{0} m_{s}^{a s q}$ | $L / a$ | $T / a$ | $N_{\text {conf }} \times N_{t}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | $2.152(5)$ | 0.0097 | 0.0484 | 16 | 48 | $631 \times 2$ |
| 2 | $2.618(3)$ | 0.01 | 0.05 | 20 | 64 | $595 \times 2$ |
| 3 | $3.699(3)$ | 0.0062 | 0.031 | 28 | 96 | $566 \times 4$ |
| 4 | $5.296(7)$ | 0.0036 | 0.018 | 48 | 144 | $201 \times 2$ |
| 5 | $7.115(20)$ | 0.0028 | 0.014 | 64 | 192 | $208 \times 2$ |

TABLE I: Ensembles (sets) of MILC configurations used for this analysis. The sea asqtad quark masses $m_{l}^{a s q}(l=u / d)$ and $m_{s}^{a s q}$ are given in the MILC convention where $u_{0}$ is the plaquette tadpole parameter. The lattice spacing values in units of $r_{1}$ after 'smoothing' are given in the second column [13]. Set 1 is 'very coarse'; set 2 , 'coarse'; set 3 , 'fine'; set 4 'superfine' and set 5 'ultrafine'. The size of the lattices is given by $L^{3} \times T$. The final column gives the number of configurations used and the number of time sources for propagators per configuration.

## II. LATTICE CALCULATION

We use ensembles of lattice gluon configurations at 5 different, widely separated, values of the lattice spacing, provided by the MILC collaboration. The configurations include the effect of $u, d$ and $s$ quarks in the sea with the improved staggered (asqtad) formalism. Table $\square$ lists the parameters of the ensembles. The $u$ and $d$ masses are taken to be the same, and the ensembles have $m_{u / d} / m_{s}$ approximately 0.2 . As discussed in section I, we expect sea quark mass effects to be small for the gold-plated mesons with no valence light quarks that we study here.

The lattice spacing is determined on an ensemble-byensemble basis using a parameter $r_{1}$ that comes from fits to the static quark potential calculated on the lattice [13]. This parameter can be determined with very small statistical/fitting errors. However, its physical value is not accessible to experiment and so must be determined using other quantities, calculated on the lattice, that are. We have determined $r_{1}=0.3133(23) \mathrm{fm}$ using four different quantities ranging from the $(2 \mathrm{~S}-1 \mathrm{~S})$ splitting in the $\Upsilon$ system to the decay constant of the $\eta_{s}$ (fixing $f_{K}$ and $f_{\pi}$ from experiment) [14]. Using our value for $r_{1}$ and the MILC values for $r_{1} / a$ given in Table we can determine $a$ in fm on each ensemble or, equivalently, $a^{-1}$ in GeV needed to convert lattice masses to physical units. It is important to note that the relative values of $a$ (from $\left.r_{1} / a\right)$ are determined more accurately than the absolute values of $a$ (from $r_{1}$ ). Our fits account for this to give two separate errors in our error budgets.

Table $\square$ lists the number of configurations used from each ensemble and the number of time sources for the valence HISQ propagators per configuration. To increase statistics further we use a 'random wall' source for the quark propagators from a given time source. When quark propagators are combined this effectively increases the number of meson correlators sampled and reduces the statistical noise by a large factor for the case of pseudoscalar mesons. We also take a random starting point for our time sources for the very coarse, coarse and fine
ensembles.
We use many different masses for the HISQ valence quarks varying from masses close to that of the $s$ quark to much heavier values for $c$ quarks and for quarks with masses between $c$ and $b$. On all sets the largest valence quark mass in lattice units that we use is $m_{h} a=0.85$. These propagators are combined to make goldstone pseudoscalar meson correlators at zero momentum with all possible combinations of valence quark masses. We separate them into 'heavy-heavy' correlators when both masses are the same and are close to charm or heavier; 'heavy-charm' when one mass is close to charm and the other is heavier and 'heavy-strange' when one mass is close to strange and the other is close to charm or heavier.

The meson correlation function is averaged over time sources on a single configuration so that any correlations between the time sources are removed. Autocorrelations between results on successive configurations in an ensemble were visible by binning only on the finest lattices. We therefore bin the correlators on superfine and ultrafine lattices by a factor of two.

The meson correlators are fit as a function of the time separation between source and sink, $t$, to the form:

$$
\begin{equation*}
\bar{C}(t)=\sum_{i} a_{i}\left(e^{-M_{i} t}+e^{-M_{i}(T-t)}\right) \tag{1}
\end{equation*}
$$

for the case of equal mass quark and antiquark. $i=1$ is the ground state and larger $i$ values denote radial or other excitations with the same $J^{P C}$ quantum numbers. $T$ is the time extent of the lattice. For the unequal mass case there are additional 'oscillating' terms coming from opposite parity states, denoted $i_{p}$ :

$$
\begin{equation*}
\bar{C}(t)=\sum_{i, i_{p}} a_{i} e^{-M_{i} t}+(-1)^{t} a_{i_{p}} e^{-M_{i_{p}} t}+(t \rightarrow T-t) \tag{2}
\end{equation*}
$$

To fit we use a number of exponentials $i$, and where appropriate $i_{p}$, in the range $2-6$, loosely constraining the higher order exponentials by the use of Bayesian priors [15]. As the number of exponentials increases, we see the $\chi^{2}$ value fall below 1 and the results for the fitted values and their errors for the parameters for the ground state $i=1$ stabilise. This allows us to determine the ground state parameters $a_{1}$ and $M_{1}$ as accurately as possible whilst allowing the full systematic error from the presence of higher excitations in the correlation function. We take the fit parameters to be the logarithm of the ground state masses $M_{1}$ and $M_{1_{p}}$ and the logarithms of the differences in mass between successive radial excitations (which are then forced to be positive). The Bayesian prior value for $M_{1}$ is obtained from a simple 'effective mass' in the correlator and the prior width on the value is taken as a factor of 1.5 . The prior value for the mass splitting between higher excitations is taken as roughly 600 MeV with a width of 300 MeV . Where oscillating states appear in the fit, the prior value for $M_{1_{p}}$ is taken as roughly 600 MeV above $M_{1}$ with a prior width of

300 MeV and the splitting between higher oscillating excitations is taken to be the same as for the non-oscillating states. The amplitudes $a_{i}$ and $a_{i_{p}}$ are given prior widths of 1.0 . We apply a cut on the range of eigenvalues from the correlation matrix that are used in the fit of $10^{-3}$ or $10^{-4}$. We also cut out very small $t$ values from our fit, typically below 3 or 4 , to reduce the effect of higher excitations.

The amplitude, $a_{1}$, from the fits in equations (1) and $(2)$ is directly related to the matrix element for the local pseudoscalar operator to create or destroy the groundstate pseudoscalar meson from the vacuum. Using the PCAC relation this can be related to the matrix element for the temporal axial current and thence to the decay constant. The PCAC relation guarantees that no renormalisation of the decay constant is needed. We have:

$$
\begin{equation*}
f_{P}=\left(m_{a}+m_{b}\right) \sqrt{\frac{2 a_{1}}{M_{1}^{3}}} \tag{3}
\end{equation*}
$$

for meson $P$. Here $m_{a}$ and $m_{b}$ are the quark masses used in the lattice QCD calculation.
$f_{P}$ is clearly a measure of the internal structure of a meson and in turn is related, for charged pseudoscalars such as the $\pi, K, D, D_{s}, B$ and $B_{c}$ mesons, to the experimentally measurable leptonic branching fraction via a $W$ boson:

$$
\begin{equation*}
\mathcal{B}\left(P \rightarrow l \nu_{l}(\gamma)\right)=\frac{G_{F}^{2}\left|V_{a b}\right|^{2} \tau_{P}}{8 \pi} f_{P}^{2} m_{l}^{2} m_{P}\left(1-\frac{m_{l}^{2}}{m_{P}^{2}}\right)^{2} \tag{4}
\end{equation*}
$$

up to calculable electromagnetic corrections. $V_{a b}$ is the appropriate CKM element for quark content $a \bar{b}, \tau_{P}$ is the pseudoscalar meson lifetime. For neutral mesons there is no possibility to annihilate to a single particle via the temporal axial current. However, in the Standard Model the $B_{s}$ and $B$ are expected to annihilate to $\mu^{+} \mu^{-}$with a rate that is proportional to $f_{P}^{2}\left|V_{t b}^{*} V_{t q}\right|^{2}$ via 4 -fermion operators in the effective weak Hamiltonian [16]. For the heavy-heavy pseudoscalar, the decay rate to two photons is related to its decay constant but only at leading order in a nonrelativistic expansion. In section III we compare the pseudoscalar decay constant to that of its associated vector meson, determined directly from its decay to leptons.

The results for masses and decay constants from fits in eqs. (1) and (2) and using eq. (3) are in units of the lattice spacing, and given in this form in the tables of section III. To convert to physical units, as discussed earlier, we determine the lattice spacing using the parameter $r_{1}$.

We then fit the results in physical units as a function of heavy quark mass to determine the heavy quark mass dependence and the physical value at the $b$ quark mass. Because the bare heavy quark mass used in the lattice action runs with lattice spacing we need a proxy for it that is a physical quantity, such as a meson mass. In 4] we used the heavy-strange pseudoscalar mass since we were focussing on heavy-strange mesons. Here we choose

| electromagnetism $c$-in-sea |  |  |  |
| :--- | :---: | :---: | :---: |
| $M_{\eta_{b}}$ | $-1.6(8)$ | $-5(3)$ | $-2.4(2.4)$ |
| $M_{\eta_{c}}$ | $-2.6(1.3)$ | $-0.4(2)$ | $-2.4(1.2)$ |
| $M_{B_{c}}$ | $+2(1)$ | $-1(1)$ | - |
| $M_{B_{s}}$ | $-0.1(1)$ | - | - |
| $M_{D_{s}}$ | $+1.3(7)$ | - | - |

TABLE II: Estimates of shifts in MeV to be applied to the masses determined in lattice QCD to allow for missing electromagnetism, $c$ quarks in the sea and annihilation to gluons for the $\eta_{b}$ and $\eta_{c}$ mesons [10, 18]. The electromagnetic shift is estimated from a potential model for $\eta_{b}, \eta_{c}$ and $B_{c}$ and from a comparison of charged and neutral meson masses for $B_{s}$ and $D_{s}$. The $c$-in-sea and gluon annihilation shifts are estimated from perturbation theory. The errors on the shifts are given in brackets. Note that for the $\eta_{S}$ there are no shifts because the mass is fixed in lattice QCD [14].
the mass of the heavy-heavy pseudoscalar meson, $\eta_{h}$, to provide the same $x$-axis for all of our plots showing dependence on the heavy quark mass. The positions of $c$ and $b$ on these plots are then determined by the values of the $\eta_{c}$ and $\eta_{b}$ masses.

The experimental results for the $\eta_{b}$ and $\eta_{c}$ meson masses are $9.391(3) \mathrm{GeV}$ and $2.981(1) \mathrm{GeV}$ respectively [17. Our lattice QCD calculation, however, is missing some ingredients from the real world which means that we must adjust the experimental values we use in our calibration. The key missing ingredients are electromagnetism, $c$ quarks in the sea and the possibility for the $\eta_{b}$ and $\eta_{c}$ mesons to annihilate to gluons, which we do not allow for in determining our $\eta_{c}$ and $\eta_{b}$ correlators. These effects all act in the same direction, that of lowering the meson mass in the real world compared to that in our lattice QCD world. We estimate the total shift from these effects for the $\eta_{c}$ to be $-5.4(2.7) \mathrm{MeV}$ and for the $\eta_{b}$, as $-9(6) \mathrm{MeV}$ [18]. The appropriate 'experimental' masses for the $\eta_{c}$ and $\eta_{b}$ for our calculations are then $2.986(3) \mathrm{GeV}$ and $9.400(7) \mathrm{GeV}$.

Since we need to allow for the three ingredients missing from our lattice QCD calculation when we determine meson masses in section III, we give in Table II a summary of our estimates of these effects [10, 18]. These estimates will be used to shift the lattice QCD results for comparison to experiment. Effects on decay constants are much smaller and we do not apply shifts in that case but simply include an additional uncertainty in the error budget.

For consistency we fit a similar functional form to all quantities. This form must take account of physical heavy quark mass-dependence; discretisation errors and, for heavy-charm and heavy-strange mesons, mistuning of $c$ and $s$ quark masses. We use the standard constrained fitting techniques that we earlier applied to the correlators [15]. For the dependence on heavy quark mass and

|  | form of $f_{0}$ | $b$ | $A$ | $c_{0000}$ | $c_{i j k l}$ |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $f_{\eta_{h}}$ | $A\left(M / M_{0}\right)^{b}$ | $0 \pm 1$ | $0 \pm 2$ | 1 | $0 \pm 4.5$ |
| $\Delta_{H_{s}, h h}$ | $A\left(M / M_{0}\right)^{b}$ | 1 | 1 | $0 \pm 2$ | $0 \pm 1.5$ |
| $f_{H_{s}}$ | $A\left(\frac{\alpha_{V}(M)}{\alpha_{V}\left(M_{\eta_{c}}\right)}\right)^{-2 / 9}\left(\frac{M}{M_{0}}\right)^{b}$ | -0.5 | $0 \pm 2$ | 1 | $0 \pm 1.5$ |
| $\Delta_{H_{c}, h h}$ | $A\left(\left(M\left(-M_{\eta_{c}}\right) / M_{0}\right)^{b}\right.$ | 1 | 1 | $0 \pm 2$ | $0 \pm 1.5$ |
| $f_{H_{c}}$ | $A\left(\frac{\alpha_{V}(M)}{\alpha_{V}\left(M_{\eta_{c}}\right)}\right)^{-2 / 9}\left(\frac{M}{M_{0}}\right)^{b}$ | -0.5 | $0 \pm 2$ | 1 | $0 \pm 3$ |
| $\Delta_{H_{c}, h s}$ | $A\left(M / M_{0}\right)^{b}$ | 0 | 1 | $0 \pm 2$ | $0 \pm 1.5$ |

TABLE III: The functional form for $f_{0}(M)$, the leading power dependence on the heavy quark mass, used in fitting the different quantities described in section III using equation (5). The third and fourth columns give the prior values and widths for the parameters $A$ and $b$. In most cases $b$ was fixed and then a single number is given. Likewise the sixth column gives the prior value and width for the $c_{i j k l}$ where the sum was normalised so that $c_{0000}$ was set equal to 1 .
lattice spacing for each set of results $f(M, a)$, we use

$$
\begin{align*}
& f(M, a)=f_{0}(M) \times \\
& \sum_{i=0}^{7} \sum_{j, k=0}^{3} \sum_{l=0}^{1} c_{i j k l}\left(\frac{M_{0}}{M}\right)^{i}\left(\frac{a m_{1}}{\pi}\right)^{2 j}\left(\frac{a m_{2}}{\pi}\right)^{2 k}\left(\frac{a \Lambda}{\pi}\right)^{2 l} \\
& +\delta f_{s}+\delta f_{c} \tag{5}
\end{align*}
$$

The quantity that we use for the heavy quark mass, $M$, is given by $M=M_{\eta_{h}}$. $f_{0}$ is a function giving the 'leading power' behaviour expected for each quantity. This is either derived from HQET or potential model expectations and takes the general form $A\left(M / M_{0}\right)^{b}$. For the decay constants $f_{H_{c}}$ and $f_{H_{s}}$ we multiply this by the ratio of $\alpha_{s}$ values at the $b$ and the $c$ raised to the power of $-2 / \beta_{0}=-2 / 9$ for $n_{f}=3$. This is the expected prefactor from resumming leading logarithms in HQET [19]. For $\alpha_{s}$ we take $\alpha_{V}$ from lattice QCD [3, 20. We take $M_{0}$ to have the value 2 GeV so that the factor $M_{0} / M$ is approximately $1 \mathrm{GeV} / m_{b}$. We tabulate the different forms for $f_{0}$ in Table III along with the prior values taken for $A$ and $b . b$ is allowed to float for the fit to $f_{\eta_{h}}$. In other cases it is fixed to the expected value but we have checked that allowing it to float returns the expected value within errors. We take the same prior for $A$ of $0 \pm 2$ in all cases.

The sum to the right of the leading term includes higher order corrections to the physical massdependence. These take the form of powers of $M_{0} / M$, again using $M_{0}=2 \mathrm{GeV}$. We allow for 8 terms in the sum so that there is enough leeway to describe (by Taylor's theorem) any physically reasonable functional form in the fixed mass range from $c$ to $b$. For the heavy-charm case we in fact fit from $M=4 \mathrm{GeV}$ upwards so that the functional form is that appropriate to the unequal valence mass case.

The other terms in the sum of eq. (5) allow for systematic errors resulting from sensitivity to the lattice spacing. Such discretisation errors depend on the lattice momentum cut-off, $\pi / a$, but can have a scale set by the different masses involved in the quantity under study. We allow for discretisation errors appearing with a scale of
$m_{1}$ and $m_{2}$, where $m_{1}$ and $m_{2}$ are the two quark masses in the meson (they will be the same in heavyonium). To be conservative we allow in addition further discretisation errors with a scale of $\Lambda_{\mathrm{QCD}}$ where we take $\Lambda_{\mathrm{QCD}}=$ 0.5 GeV . The powers of lattice spacing that appear in the terms must be even since discretisation errors only appear as even powers for staggered quarks. For the decay constants the $c_{i j k l}$ are normalised so that $c_{0000}=1$. For the mass differences the fits are normalised so that $A$ is 1 and $c_{0000}$ floats. This is simply so that the fit can allow for significant discretisation errors when the physical mass difference is very small (particularly for the case of the $B_{c}$ to be discussed in section III C). The prior values for the other $c_{i j k l}$ are taken to be the same for all $i, j, k$ and $l$ but vary depending on the size of discretisation errors for the quantity being fit. They are larger for heavyonium than for heavy-strange quantities, for example. The values used are tabulated in Table III.

The mistuning of the strange and charm quark masses, where relevant, can be handled very simply because our tuning of these masses is in fact very good. We simply include an additional additive factor in the fit of

$$
\begin{align*}
\delta f_{s}= & \left(c_{s}+\frac{d_{s}}{M}+e_{s}\left[\left(\frac{a m_{1}}{\pi}\right)^{2}+\left(\frac{a m_{2}}{\pi}\right)^{2}\right]\right) \times \\
& \left(m_{\eta_{s}, \text { latt }}^{2}-m_{\eta_{s}, \text { contnm }}^{2}\right) \tag{6}
\end{align*}
$$

for heavy-strange mesons and

$$
\begin{align*}
\delta f_{c}= & \left(c_{c}+\frac{d_{c}}{M}+e_{c}\left[\left(\frac{a m_{1}}{\pi}\right)^{2}+\left(\frac{a m_{2}}{\pi}\right)^{2}\right]\right) \times \\
& \left(m_{\eta_{c}, \text { latt }}-m_{\eta_{c}, \text { contnm }}\right) \tag{7}
\end{align*}
$$

for heavy-charm mesons. The forms above allow for linear quark mass dependence away from the tuned point. We do not need to include higher order terms because we are so close to the tuned point but we do allow for an $M$-dependent slope with discretisation errors (although in most cases neither of these additions makes any difference).

To tune the strange quark mass we use the $\eta_{s}$, an unphysical $s \bar{s}$ pseudoscalar meson whose valence quarks are not allowed to annihilate. Lattice QCD simulations show that its mass $m_{\eta_{s}, \text { contnm }}=0.6858(40) \mathrm{GeV}$ [14] when the strange quark mass is tuned (from the $K$ meson). Being a light pseudoscalar meson, the square of its mass is proportional to the quark mass. To tune the $c$ quark mass we use the $\eta_{c}$ meson, as discussed earlier. The $\eta_{c}$ meson is far from the light quark limit and so the meson mass is simply proportional to the quark mass. $c_{s}$ and $c_{c}$ are dimensionful coefficients that represent physical light quark mass dependence and can be compared between lattice QCD calculations and with models.

We do not include correlations between the results for different $M$ on a given ensemble. We have not measured these correlations and the empirical Bayes criterion suggests that they are small. If we include a correlation matrix by hand for the results it makes very little difference, a fraction of a standard deviation, to the final results.

| Set $m_{h} a$ | $\epsilon$ | $M_{\eta_{h}} a$ | $f_{\eta_{h}} a$ |  |
| :--- | :--- | :--- | :--- | :--- |
| 1 | 0.66 | -0.244 | $1.92020(16)$ | $0.3044(4)$ |
|  | 0.81 | -0.335 | $2.19381(16)$ | $0.3491(5)$ |
|  | 0.825 | -0.344 | $2.22013(15)$ | $0.3539(5)$ |
|  | 0.85 | -0.359 | $2.26352(15)$ | $0.3622(5)$ |
| 2 | 0.44 | -0.12 | $1.42402(13)$ | $0.21786(21)$ |
|  | 0.63 | -0.226 | $1.80849(11)$ | $0.25998(20)$ |
|  | 0.66 | -0.244 | $1.86666(10)$ | $0.26721(20)$ |
|  | 0.72 | -0.28 | $1.98109(10)$ | $0.28228(22)$ |
|  | 0.753 | -0.3 | $2.04293(10)$ | $0.29114(24)$ |
|  | 0.85 | -0.36 | $2.21935(10)$ | $0.31900(27)$ |
| 3 | 0.3 | -0.06 | $1.03141(8)$ | $0.15205(11)$ |
|  | 0.413 | -0.107 | $1.28057(7)$ | $0.17217(11)$ |
|  | 0.43 | -0.115 | $1.31691(7)$ | $0.17508(11)$ |
|  | 0.44 | -0.12 | $1.33816(7)$ | $0.17678(11)$ |
|  | 0.45 | -0.125 | $1.35934(7)$ | $0.17850(11)$ |
|  | 0.7 | -0.27 | $1.86536(5)$ | $0.22339(12)$ |
|  | 0.85 | -0.36 | $2.14981(5)$ | $0.25658(12)$ |
| 4 | 0.273 | -0.0487 | $0.89935(10)$ | $0.11864(24)$ |
|  | 0.28 | -0.051 | $0.91543(8)$ | $0.11986(21)$ |
|  | 0.564 | -0.187 | $1.52542(6)$ | $0.16004(16)$ |
|  | 0.705 | -0.271 | $1.80845(6)$ | $0.18071(16)$ |
|  | 0.76 | -0.305 | $1.91567(6)$ | $0.18962(17)$ |
|  | 0.85 | -0.359 | $2.08753(6)$ | $0.20576(16)$ |
| 5 | 0.193 | -0.0247 | $0.66628(13)$ | $0.0882(3)$ |
|  | 0.195 | -0.02525 | $0.67117(6)$ | $0.08846(11)$ |
|  | 0.4 | -0.101 | $1.13276(7)$ | $0.1149(4)$ |
|  | 0.5 | -0.151 | $1.34477(8)$ | $0.1260(5)$ |
|  | 0.7 | -0.268 | $1.75189(7)$ | $0.1498(5)$ |
|  | 0.85 | -0.359 | $2.04296(7)$ | $0.1708(6)$ |

TABLE IV: Results for the masses and decay constants in lattice units of the goldstone pseudoscalars made from valence HISQ heavy quarks on the different MILC ensembles, enumerated in Table Columns 2 and 3 give the corresponding bare heavy quark mass and the $\epsilon$ parameter, calculated at tree-level in $m_{h} a$ [10]. This corresponds to a coefficient for the Naik 3 -link discretisation correction of $1+\epsilon$. Meson masses from fitting these correlators using a simpler fitting form are given in [3]. Results given here are in agreement but somewhat more accurate. The results for heavy quark masses close to charm are also given in [10.

We also do not include effects from sea quark massdependence but, based on earlier work [10, we are able to estimate an uncertainty for that in our final results.

## III. RESULTS

## A. $f_{\eta_{b}}$

The correlators for pseudoscalar heavyonium mesons have very little noise and we can readily obtain groundstate masses with statistical errors in the fourth or fifth decimal place and ground-state decay constants with errors of $0.1 \%$. Our results on each ensemble are given in Table IV

Results for $f_{\eta_{h}}$ are plotted against $M_{\eta_{h}}$ in Figure 1. Discretisation errors are apparent in this plot and lead


FIG. 1: Results for the pseudoscalar heavyonium decay constant plotted as a function of the pseudoscalar heavyonium mass. Results for very coarse, coarse, fine, superfine and ultrafine lattices appear from left to right. The colored dashed lines give the fitted function for that lattice spacing. The black line with grey error band gives the physical curve derived from our fit. The black circles with error bars at $M_{\eta_{c}}$ and $M_{\eta_{b}}$ are the values for the heavyonium vector decay constant at these physical points derived from the experimental leptonic widths for the $J / \psi$ and $\Upsilon$. The left-most black circle corresponds to the fictitious pseudoscalar $\eta_{s}$ particle whose decay constant was determined in 14 .
to results at each value of the lattice spacing deviating substantially from the physical curve as the quark mass is increased. We fit the results to a physical curve allowing for discretisation errors as a function of the mass, as described in section $\Pi$ and using the priors from Table III. The power, $b$, in eq. (5) is allowed to float in the fit.

The obvious approach from which to gain some physical insight in this case is that of the nonrelativistic potential model. In its simplest form this involves solving Schrödinger's equation for the wavefunction of a twoparticle system with reduced mass $\mu\left(=m_{b} / 2\right.$ for two $b$ quarks) in a potential $V(r)$ which is a function of the radial separation, $r$. At short distances we expect a Coulomb-like potential from QCD, and at large distances a string-like linear potential. However, other phenomenological forms that interpolate between these two at intermediate distances also work well at reproducing the bound-state spectrum, see for example [21]. The wavefunction is useful for a first approximation in calculations of transition rates. In this sense, the wavefunction at the origin, $\psi(0)$, can be related to the decay constant by $\psi(0)=f_{\eta_{h}} \sqrt{M_{\eta_{h}} / 12}$. However, $\psi(0)$ must be renormalised before it can be related to a physical matrix element and some of the radiative corrections are very substantial 21. In addition values of $\psi(0)$ vary widely with different forms for the potential that reproduce the same bound state spectrum because the spectrum itself provides little constraint on the potential at short distances [22]. Here we will make comparisons of our lattice

QCD results to those from potential models but it is important to realise that the lattice QCD results for decay constants represent well-defined matrix elements in QCD and not model calculations.

For a potential model with potential $r^{N}$ power counting arguments yield $\psi(0) \propto \mu^{3 /(4+2 N)}$ (see, for example, [23]). Then we would expect our fit for $f_{\eta_{h}}$ to need $b=1$ for $N=-1$ but $b=0$ for $N=1$, the two extremes of the QCD heavy quark potential. Simply from comparing values at $c$ and $b$ we might infer $b \approx 0.5$. In fact our fit gives the result $b=-0.08(10)$ but with significant power corrections in $1 / M$, so that a simple power in $M$ does not describe the results using our parameterisation. The physical curve that we extract of dependence on the heavyonium meson mass is shown as the grey band in Figure 1.

The fit has $\chi^{2}$ of 1.2 for 29 degrees of freedom and allows us to extract results for $c$ and $b$ quarks. The result for $f_{\eta_{c}}$ agrees within $1 \sigma$ with our earlier result of $0.3947(22) \mathrm{GeV}$ [10] where we fit results at $c$ only but included additional ensembles at different values of the sea $u / d$ quark masses. Results for $b$ quarks give:

$$
\begin{align*}
f_{\eta_{b}} & =0.667(6)(2) \mathrm{GeV} \\
f_{\eta_{b}} / f_{\eta_{c}} & =1.698(13)(5) \tag{8}
\end{align*}
$$

The first error comes from the fit and the second from additional systematic errors from effects not included in our lattice QCD calculation, i.e. electromagnetism, $c$ quarks in the sea and (since we have not extrapolated to physical $u / d$ sea quark masses here) sea quark mass effects. Both errors are split into their component parts in the error budget of Table V. We estimated the effects of electromagnetism on $f_{\eta_{c}}$ from a potential model in [10. We take the same $0.4 \%$ error for $f_{\eta_{b}}$ since it is a more tightly bound particle but with smaller electromagnetic charges. There is then some cancellation of the effect in the ratio $f_{\eta_{b}} / f_{\eta_{c}}$. The effects of $c$ quarks in the sea were shown to be similar to that of the hyperfine potential in 10 and the effect on $f_{\eta_{h}}$ can then be estimated from the difference between $f_{\eta_{h}}$ and its associated vector particle. This is very small as we show below. We therefore expect that missing $c$ in the sea has a negligible effect on $f_{\eta_{c}}$ and we estimate $0.2 \%$ on $f_{\eta_{b}}$ where it is magnified by $\left(m_{b} / m_{c}\right)^{2}$. Sea quark mass effects on $f_{\eta_{c}}$ were shown to be very small in [10], at the same level as the statistical errors of $0.1 \%$. For $f_{\eta_{b}}$ we expect even smaller effects because it is a smaller particle. We take a $0.1 \%$ error nevertheless, but allow for some cancellation in the ratio of $f_{\eta_{b}} / f_{\eta_{c}}$.

The two rightmost black points (at $M_{\eta_{b}}$ and $M_{\eta_{c}}$ ) in Fig. 1 give the experimental values for the decay constants of the corresponding vector heavyonium mesons, $J / \psi$ and $\Upsilon$, for comparison to the results calculated here in lattice QCD for the $\eta_{c}$ and $\eta_{b}$. The decay constant for a vector meson can be defined by:

$$
\begin{equation*}
\sum_{i}<0\left|\bar{\psi} \gamma_{i} \psi\right| V_{i}>/ 3=f_{V} m_{V} \tag{9}
\end{equation*}
$$

| Error | $f_{\eta_{b}}$ | $f_{\eta_{b}} / f_{\eta_{c}}$ |
| :--- | :---: | :---: |
| statistics | 0.6 | 0.6 |
| $M$ extrapoln | 0.2 | 0.1 |
| $a^{2}$ extrapoln | 0.5 | 0.4 |
| $r_{1}$ | 0.4 | 0.1 |
| $r_{1} / a$ | 0.5 | 0.3 |
| $M_{\eta_{c}}$ | 0.00 | 0.05 |
| sea quark mass effects | 0.1 | 0.05 |
| electromagnetism | 0.4 | 0.2 |
| $c$ in the sea | 0.2 | 0.2 |
| Total $(\%)$ | 1.0 | 0.9 |

TABLE V: Full error budget for $f_{\eta_{b}}$ and the ratio $f_{\eta_{b}} / f_{\eta_{c}}$ in $\%$. See text for a fuller description of each error. The total error is obtained by adding the individual errors in quadrature.

It has the advantage here that it can be extracted very accurately from experiment because vector heavyonium mesons can annihilate, through the vector currrent, to a photon, seen as two leptons in the final state. The relationship between the leptonic decay width and the decay constant is:

$$
\begin{equation*}
\Gamma\left(V_{h} \rightarrow e^{+} e^{-}\right)=\frac{4 \pi}{3} \alpha_{Q E D}^{2} e_{h}^{2} \frac{f_{V}^{2}}{m_{V}} \tag{10}
\end{equation*}
$$

where $e_{h}$ is the electric charge of the heavy quark in units of $e$. The experimental results [17] give $f_{J / \psi}=407(5)$ MeV and $f_{\Upsilon}=689(5) \mathrm{GeV}$, remembering that the electromagnetic coupling constant runs with scale and using $1 / \alpha_{Q E D}\left(m_{c}\right)=134$ and $1 / \alpha_{Q E D}\left(m_{b}\right)=132[24$. Thus $1 \%$ accurate results for this decay constant are available from experiment, and can be used to test lattice QCD. Lattice QCD calculations of the $\Upsilon$ decay constant can be done [25] but they are not yet as accurate as the results we give here for the $\eta_{b}$.

The surprising result that we find on comparing the vector decay constant from experiment to the pseudoscalar decay constant from lattice QCD is how close they are. In the nonrelativistic limit, where spin effects disappear, the vector and pseudoscalar become the same particle. Away from this point, however, there can be substantial relativistic corrections, particularly for charmonium. Instead we find that the pseudoscalar decay constant is $3 \%$ lower than the vector in both cases with an error of 1-2\%.

Unfortunately this cannot be directly tested through decay modes of the $\eta_{c}$ or $\eta_{b}$. The decay rate to two photons is indirectly related to the decay constant as the leading term in a nonrelativistic approximation:

$$
\begin{equation*}
\Gamma\left(\eta_{h} \rightarrow \gamma \gamma\right)=\frac{12 \pi e_{h}^{4} \alpha_{Q E D}^{2}|\psi(0)|^{2}}{m_{h}^{2}} \tag{11}
\end{equation*}
$$

This formula has radiative and relativistic corrections at the next order. The decay width is not known for the $\eta_{b}$ and only very poorly known for the $\eta_{c}$, with the Particle Data Group estimate given as $7.2(2.1) \mathrm{keV}$ [17]. Substi-
tuting this into eq. (11) and taking $m_{c}=M_{\eta_{c}} / 2$, justifiable at this order, gives $f_{\eta_{c}}=0.4(1) \mathrm{GeV}$, where only the large error from experiment is shown. This is consistent with our value but much less accurate so does not provide a useful test.

As discussed earlier, a direct comparison of lattice QCD results for $f_{\eta_{h}}$ and potential model values for $\psi(0)$ is not particularly useful. Values for $\psi(0)$ for the ground state in bottomonium vary by a factor of 1.5 for different forms for the potential in [22]. This variation is reduced somewhat, and radiative corrections cancel, if we compare the ratio of values at $b$ and $c$. Here the lattice QCD result above of 1.698(14) favours the strong variation of $\psi(0)$ with quark mass seen in the Cornell potential. For this potential [22] gives a ratio $\psi_{b}(0) / \psi_{c}(0)$ of 3.1 , yielding a decay constant ratio of 1.8 .

Figure 1 also includes as the leftmost black point a value for the decay constant of the $\eta_{s}$ as determined from lattice QCD [14. Although our fit becomes unstable below $M$ of 2 GeV , it is interesting to see that $f_{\eta_{s}}$ does not look out of place on this plot as the light and heavy sectors are smoothly connected together.

## B. $m_{B_{s}}$ and $f_{B_{s}}$

Our calculations for heavy-strange mesons were described in [4] and so we only add briefly to that discussion here. In Table VI we give our full set of results, including values at a variety of strange quark masses for completeness. In [4] we used the heavy-strange mass itself as a proxy for the heavy quark mass and obtained good agreement for the mass of the $B_{s}$ with experiment and a value for $f_{B_{s}}$ of $225(4) \mathrm{MeV}$.

Here, for consistency with the other calculations, we use instead $M_{\eta_{h}}$ for the heavy quark mass and the fit form given in eq. (5). For the heavy-strange meson mass, as in [4], we fit to the mass difference:

$$
\begin{equation*}
\Delta_{H_{s}, h h}=m_{H_{s}}-\frac{m_{\eta_{h}}}{2} \tag{12}
\end{equation*}
$$

We take account of mistuning of the strange quark mass using the factor given in eq. (6). For the decay constant fit we fix the power of the leading $M$-dependence, $b=$ -0.5 . Allowing $b$ to float gives results for $b$ in agreement with this value to within $20 \%$.

Our fit to $\Delta_{H_{s}, h h}$ a is shown in Figure 2 and gives $\chi^{2}=0.2$ for 17 degrees of freedom. The values extracted at the $c$ and $b$ masses agree well, within $1 \sigma$, with our earlier results [4, 10]. When account is taken of electromagnetic and other effects missing in the lattice calculation these earlier results translate into values for $m_{D_{s}}=1.969(3) \mathrm{GeV}$ [10] and $m_{B_{s}}=5.358(12) \mathrm{GeV}$ 4]. The increased error at the $b$ results from increased statistical and discretisation errors for heavier quark masses as well as the extrapolation in $M$. Our result for $m_{B_{s}}$ agrees within the 12 MeV error with that determined from full lattice QCD using a completely different

| Set | $m_{s} a$ | $M_{\eta_{s}} a$ | $m_{h} a$ | $M_{H_{s}} a$ | $f_{H_{s}} a$ |
| :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0.061 | 0.50490(36) | 0.66 | 1.3108(6) | 0.1913(7) |
|  |  |  | 0.81 | 1.4665(8) | 0.1970(10) |
|  | 0.066 | 0.52524(36) | 0.66 | 1.3164(5) | 0.1929(7) |
|  |  |  | 0.825 | 1.4869(7) | 0.1994(10) |
| 2 | 0.0492 | 0.41436(23) | 0.44 | 0.9850(4) | 0.1500(5) |
|  |  |  | 0.63 | 1.2007(5) | 0.1559(7) |
|  |  |  | 0.85 | 1.4289(8) | $0.1613(10)$ |
|  | 0.0546 | 0.43654(24) | 0.44 | 0.9915(4) | 0.1516(5) |
|  |  |  | 0.66 | 1.2391(5) | 0.1586(6) |
|  |  |  | 0.85 | 1.4348(7) | 0.1634(9) |
| 3 | 0.0337 | 0.29413(12) | 0.3 | 0.70845(17) | 0.1054(2) |
|  |  |  | 0.413 | 0.84721(23) | 0.1084(2) |
|  |  |  | 0.7 | 1.1660(4) | 0.1112(5) |
|  |  |  | 0.85 | 1.3190(5) | 0.1123(6) |
|  | 0.0358 | 0.30332(12) | 0.3 | 0.71119(16) | 0.1061(2) |
|  |  |  | 0.43 | 0.86982(23) | 0.1094(2) |
|  |  |  | 0.44 | 0.88152(23) | 0.1096(3) |
|  |  |  | 0.7 | 1.1684(4) | 0.1121(4) |
|  |  |  | 0.85 | 1.3214(5) | 0.1131(6) |
|  | 0.0366 | 0.30675(12) | 0.3 | 0.71223(16) | 0.1063(2) |
|  |  |  | 0.43 | 0.87079(22) | 0.1097(2) |
|  |  |  | 0.44 | 0.88249(23) | 0.1099(3) |
|  |  |  | 0.7 | 1.1694(4) | 0.1124(4) |
|  |  |  | 0.85 | 1.3223(5) | 0.1135(6) |
| 4 | 0.02280 .20621 (19) |  | 0.273 | 0.59350(24) | 0.0750(3) |
|  |  |  | 0.564 | 0.9313(5) | 0.0754(6) |
|  |  |  | 0.705 | 1.0811(8) | 0.0747(8) |
|  |  |  | 0.85 | 1.2279(10) | 0.0742(10) |
| 5 | $0.01610 .15278(28)$ |  | 0.193 | 0.43942(33) | 0.0553(4) |
|  |  |  | 0.5 | 0.8027(10) | 0.0541(12) |
|  |  |  | 0.7 | 1.0152(18) | 0.0513(22) |
|  |  |  | 0.85 | 1.1657(24) | 0.0495(30) |
|  | 0.0165 | 0.15484(14) | 0.195 | 0.44270(28) | 0.0555(3) |
|  |  |  | 0.5 | 0.8038(8) | 0.0546(11) |
|  |  |  | 0.7 | 1.0169(12) | 0.0526(16) |
|  |  |  | 0.85 | 1.1684(16) | 0.0517(21) |

TABLE VI: Results for the masses and decay constants in lattice units of the goldstone pseudoscalars made from valence HISQ heavy quarks with valence HISQ strange quarks on the different MILC ensembles, enumerated in Table प Column 2 gives the $s$ mass in lattice units, with several values on some ensembles around the correctly tuned value. Column 3 gives the corresponding mass for the goldstone pseudoscalar made from the $s$ quarks, which is used for tuning. Column 4 gives the heavy quark mass. The corresponding values of the Naik coefficient are given in Table IV. Many of these results were given earlier in 4, 10.
method (NRQCD) for the $b$ quark [18] with very different systematic errors, providing a stringent test of lattice QCD. Our results also agree well with experiment [17] ( $m_{D_{s}}=1.968 \mathrm{GeV}$ and $m_{B_{s}}=5.367 \mathrm{GeV}$ ) and this provides a very strong test of QCD.

The fit to the decay constant, $f_{H_{s}}$, is shown in Figure 3 and gives $\chi^{2}=0.3$ for 17 degrees of freedom. Again results at the $b$ and $c$ agree within $1 \sigma$ with our earlier results which are: $f_{D_{s}}=0.2480(25) \mathrm{GeV}$ [10] and $f_{B_{s}}=$ $0.225(4) \mathrm{GeV}$ [4].

Figures 2 and 3 give the physical fit curves as a func-


FIG. 2: Results for the difference, $\Delta_{H_{s}, h h}$ between the heavystrange pseudoscalar meson mass and one half of the pseudoscalar heavyonium mass. Results for very coarse, coarse, fine, superfine and ultrafine lattices appear from left to right. The lattice QCD results have been adjusted for slight mistuning of the $s$ quark mass. The colored dashed lines give the fitted function for that lattice spacing. The black dashed line with grey error band gives the physical curve derived from our fit. The black circles with error bars at $M_{\eta_{c}}$ and $M_{\eta_{b}}$ are the experimental values adjusted for the effects from electromagnetism, $\eta_{b} / \eta_{c}$ annihilation and $c$ quarks in the sea, none of which is included in the lattice QCD calculation.


FIG. 3: Results for the pseudoscalar heavy-strange decay constant plotted as a function of the pseudoscalar heavyonium mass. Results for very coarse, coarse, fine, superfine and ultrafine lattices appear from left to right. The lattice QCD results have been adjusted for slight mistuning of the $s$ quark mass. The colored dashed lines give the fitted function for that lattice spacing. The black dashed line with grey error band gives the physical curve derived from our fit.
tion of $M_{\eta_{h}}$. As expected, the curves are very similar to those in [4] since to a large extent the change is simply a rescaling of the $x$-axis. However they provide a consistency check that the parameterisation we use here, taking a different quantity to represent the heavy quark mass, works just as well.

| Set $m_{c} a$ | $m_{h} a$ | $M_{H_{c}} a$ | $f_{H_{c}} a$ |  |
| :--- | :--- | :--- | :--- | :--- |
| 2 | 0.63 | 0.85 | $2.01651(10)$ | $0.2854(2)$ |
| 3 | 0.413 | 0.7 | $1.57733(7)$ | $0.1916(2)$ |
|  |  | 0.85 | $1.72373(6)$ | $0.2004(1)$ |
|  | 0.43 | 0.7 | $1.59489(7)$ | $0.1938(2)$ |
|  |  | 0.85 | $1.74105(6)$ | $0.2030(1)$ |
|  | 0.44 | 0.7 | $1.60522(6)$ | $0.1952(1)$ |
|  |  | 0.85 | $1.75122(6)$ | $0.2044(1)$ |
| 4 | 0.273 | 0.564 | $1.21799(8)$ | $0.1329(2)$ |
|  |  | 0.705 | $1.36350(8)$ | $0.1367(2)$ |
|  |  | 0.76 | $1.41872(8)$ | $0.1380(2)$ |
|  |  | 0.85 | $1.50727(8)$ | $0.1402(2)$ |
|  | 0.28 | 0.564 | $1.22562(8)$ | $0.1338(2)$ |
|  |  | 0.705 | $1.37103(8)$ | $0.1376(2)$ |
|  |  | 0.76 | $1.42621(9)$ | $0.1390(2)$ |
|  |  | 0.85 | $1.51471(9)$ | $0.1413(2)$ |
| 5 | 0.195 | 0.4 | $0.90566(8)$ | $0.0967(3)$ |
|  |  | 0.5 | $1.01457(9)$ | $0.0985(4)$ |
|  |  | 0.7 | $1.22392(10)$ | $0.1005(4)$ |
|  |  | 0.85 | $1.37366(10)$ | $0.1018(5)$ |

TABLE VII: Results for the masses and decay constants in lattice units of the goldstone pseudoscalars made from valence HISQ heavy quarks with valence HISQ charm quarks on the different MILC ensembles, enumerated in Table $\mathbb{1}$ Set 1 is missing because $m_{c} a$ is already close to the highest heavy quark mass that we use. Column 2 gives the $c$ mass in lattice units, with several values on some ensembles around the tuned $c$ mass, and column 3 the heavy quark mass. The corresponding values of the Naik coefficient are given in Table IV

$$
\text { C. } \quad m_{B_{c}} \text { and } f_{B_{c}}
$$

Heavy-charm mesons are of interest because a family of gold-plated $b \bar{c}$ mesons exists of which only one, the pseudoscalar $B_{c}$ [26, 27], has been seen. Traditionally these particles have been viewed as further examples, beyond $b \bar{b}$ and $c \bar{c}$, of a heavy-heavy system and therefore a test of our understanding of this area. $b \bar{c}$ mesons, however, have a lot in common with heavy-light systems. In fact they provide a bridge between heavy-heavy and heavylight and so test our contol of QCD much more widely. The more accurately we can do these tests, the better they are.

Lattice QCD calculations of the $B_{c}$ mass can be done very accurately. Indeed the mass of the $B_{c}$ was predicted ahead of experiment with a 22 MeV error 28 using NRQCD for the $b$ quark and the 'Fermilab' clover action for the $c$ quark. The error was later reduced to 10 MeV by using a more highly improved action, HISQ, for the charm quark 18. Here we use the HISQ action for both the $c$ quark and the heavier quark up to the $b$ mass to obtain results in a completely different heavy quark formalism. In addition we calculate the decay constant of the $B_{c}$ for the first time in full lattice QCD.

To determine the $B_{c}$ mass we use the mass difference to the average of the associated heavyonium states:

$$
\begin{equation*}
\Delta_{H_{c}, h h}=M_{H_{c}}-\frac{1}{2}\left(M_{\eta_{c}}+M_{\eta_{h}}\right) \tag{13}
\end{equation*}
$$



FIG. 4: Results for the mass difference between the $H_{c}$ meson and the average of the associated heavyonium pseudoscalar meson masses plotted as a function of the pseudoscalar heavyonium mass. Results for coarse, fine, superfine and ultrafine lattices appear from left to right. The lattice QCD results have been adjusted for slight mistuning of the $c$ quark mass. The colored dashed lines give the fitted function for that lattice spacing. The black line with grey error band gives the physical curve derived from our fit. The black circle with error bar at $M_{\eta_{b}}$ gives the experimental value adjusted for the effects from electromagnetism, $\eta_{b} / \eta_{c}$ annihilation and $c$ quarks in the sea, none of which is included in the lattice QCD calculation.


FIG. 5: Results for the mass difference between the $H_{c}$ meson and the average of the associated heavyonium pseudoscalar meson masses plotted as a function of the pseudoscalar charmonium mass. Results are given for two heavy quark masses on fine lattice set 3 (pink bursts) and four heavy quark masses on superfine lattices set 4 (green crosses). Lines are drawn to guide the eye.
$\Delta_{H_{c}, h h}$ is a measure of the difference in binding energy between the symmetric heavyonium states made of $c$ and $h$ quarks and the heavyonium state made of two different mass quarks, $c$ and $h$. Here we map out $\Delta_{H_{c}, h h}$ as a function of the heavy quark mass, and reconstruct $M_{B_{c}}$ from $\Delta_{H_{c}, h h}$ determined at $h=b . \Delta_{H_{c}, h h}$ can be determined with high statistical accuracy because all of the states involved have very little noise. The fact that $\Delta_{H_{c}, h h}$ is
very small ( 0 for $m_{h}=m_{c}$ by definition and less than 100 MeV when $m_{h}=m_{b}$ ) also means that lattice errors from, for example, the uncertainty in the lattice spacing are very small. In fact, for this calculation, as discussed below, key sources of error are the uncertainties from electromagnetic, annihilation and $c$-in-the-sea shifts to the masses.

Table VII gives our results for the masses and decay constants of the $H_{c}$ mesons calculated using quark masses that are close to that of the $c$ quark mass on each ensemble and then all the heavier masses for $h$. We give results for more than one value of the $c$ quark mass on the fine and superfine ensembles (sets 3 and 4) so that slight mis-tuning in the $c$ quark mass can be corrected for. It is clear from the results that $\Delta_{H_{c}, h h}$ can be calculated with a statistical accuracy of better than 1 MeV . Errors from uncertainties in the lattice spacing are also at this level.

Figure 4 shows $\Delta_{H_{c}, h h}$ plotted against $M_{\eta_{h}}$ for the results at different values of the lattice spacing. A fairly clear linear dependence is evident. $\Delta_{H_{c}, h h}$ would be expected to increase linearly with $M_{\eta_{h}}$ at large $M_{\eta_{h}}$, in the same way as $\Delta_{H_{s}, h h}$, from a simple potential model argument. The binding energy of the $\eta_{h}$ becomes increasingly negative, roughly in proportion to $M_{\eta_{h}}$ as it increases (at least for a $r^{N}$ potential with $N=-1$ ), whilst the binding energy of the $H_{c}$ meson does not change. A corollary of this is that the dependence of $\Delta_{H_{c}, h h}$ on $M_{\eta_{c}}$ (as proxy for $m_{c}$ ) would also then be expected to be linear with a slope of opposite sign and roughly three times the magnitude. The factor of three is because the binding energy of the $\eta_{c}$ becomes more negative as $M_{\eta_{c}}$ increases, with the same dependence as the $\eta_{h}$ binding energy has on $M_{\eta_{h}}$. The $H_{c}$ binding energy will also become more negative but have double the slope because the reduced mass of the $H_{c}$ system is roughly $m_{c}$ rather than $m_{c} / 2$ for the $\eta_{c}$. On top of this $M_{\eta_{c}}$ appears halved in $\Delta_{H_{c}, h h}$.

Interestingly this factor of -3 does seem to be approximately true in comparing Figure 5, which shows the dependence of $\Delta_{H_{c}, h h}$ on $M_{\eta_{c}}$, with Figure 4. Figure 4 gives a slope of $\approx 0.012$ (over the full range) and Figure 5 gives slopes varying from -0.03 to -0.04 over a small range in $M_{\eta_{c}}$, as $M_{\eta_{h}}$ increases. In our fit to $\Delta_{H_{c}, h h}$ we include the effect of mistuning $m_{c}$ (from eq. (7)) and obtain consistent values from that.

We fit $\Delta_{H_{c}, h h}$ as a function of $M_{\eta_{h}}$ (above 4 GeV ) using the fit form described in section II. The leading mass dependence is taken to be $M_{\eta_{h}}-M_{\eta_{c}}$, so that $\Delta_{H_{c}, h h}$ vanishes when $M_{\eta_{h}}=M_{\eta_{c}}$ as it must by definition. As described in section III we include a sum of power correction terms and lattice spacing dependent terms with priors given in Table III. The fit gives $\chi^{2}$ of 0.3 for 11 degrees of freedom and result:

$$
\begin{equation*}
\Delta_{B_{c}, b b}=0.065(9) \mathrm{GeV} \tag{14}
\end{equation*}
$$

The resulting physical curve of heavy quark mass dependence is shown in grey on Figure 4. The comparison to experiment is given by the black dot with error bar at

| Error | $\Delta_{B_{c}, b b}$ | $f_{B_{c}}$ | $\Delta_{B_{c}, b s}$ |
| :--- | :---: | :---: | :---: |
| statistics | 8.4 | 0.7 | 0.5 |
| $M$ extrapoln | 3.1 | 0.2 | 0.2 |
| $a^{2}$ extrapoln | 10.9 | 0.7 | 0.4 |
| $r_{1}$ | 0.7 | 0.6 | 0.3 |
| $r_{1} / a$ | 1.4 | 0.8 | 0.3 |
| $M_{\eta_{c}}$ | 0.9 | 0.5 | 0.3 |
| sea quark mass effects | 1.5 | 0.1 | 0.1 |
| electromagnetism | $3.1^{*}$ | 0.4 | $0.2^{*}$ |
| $c$ in the sea | $5.3^{*}$ | 0.04 | $0.1^{*}$ |
| $\eta_{b, c}$ annihiln | $2.7^{*}$ | - | - |
| Total $(\%)$ | 18 | 1.6 | 0.9 |

TABLE VIII: Full error budget for $\Delta_{B_{c}, b b}, f_{B_{c}}$ and $\Delta_{B_{c}, b s}$ given as a percentage of the value. See the text for a fuller description of each error. The total error is obtained by adding the individual errors in quadrature, except for the final three systematic errors (starred) for $\Delta_{B_{c}, b b}$ and $\Delta_{B_{c}, b s}$ which are correlated and so simply added together before being combined in quadrature with the others.
$h=b$. This experimental result has been shifted to be the appropriate value to compare to our lattice QCD calculation as we now describe. The current world-average experimental result for $M_{B_{c}}-0.5\left(M_{\eta_{c}}+M_{\eta_{b}}\right)$ is $92(6)$ MeV [17]. There is a sizeable experimental error coming mainly from the $B_{c}$ but also from the $\eta_{b}$. Our lattice QCD calculation is done in a world without electromagnetism or $c$ quarks in the sea and in which the $\eta_{b}$ and $\eta_{c}$ do not annihilate. The absence of these effects (i.e. to compare to our lattice result) produces shifts to the masses as discussed in section II Estimated values for the shifts are given in Table II. The net effect is to shift the experimental value of $\Delta_{B_{c}, h h}$ down by $-8(7) \mathrm{MeV}$, where the error takes the shifts to be correlated. The 'experimental' value of $\Delta_{B_{c}, h h}$ to compare to our lattice result is then $84(9) \mathrm{MeV}$, marked on Figure 4. Our lattice result agrees with experiment, once these shifts are made, within $2 \sigma$.

From $\Delta_{B_{c}, b b}$ we can reconstruct the $B_{c}$ meson mass, now applying the shifts above to the lattice QCD calculation to obtain a result that can be compared to experiment. This gives the result

$$
\begin{equation*}
M_{B_{c}}=6.259(9)(7) \mathrm{GeV} \tag{15}
\end{equation*}
$$

Here the first error comes from the fit and the second error from the shifts applied to include missing real world effects as well as experimental uncertainties in the $\eta_{b}$ and $\eta_{c}$ masses. As can be seen, this is a sizeable part of the total error in this case. We also include in this second error an estimate of sea quark mass effects using results from [10]. There we saw no such for an equivalent quantity for $m_{D_{s}}$ within 1 MeV statistical errors and so take that as the error here. Table VIII gives the complete error budget for $\Delta_{B_{c}, b b}$ breaking down both errors into their components.

Our result for $M_{B_{c}}$ can be compared to experiment (6.277(6) GeV) and to our result from lattice QCD using a completely different formalism, NRQCD, for the $b$


FIG. 6: Results for the heavy-charm decay constant plotted as a function of the $c$ quark mass, given by the mass of the $\eta_{c}$ meson. Results are given for multiple heavy quark masses on fine lattices (pink bursts) and superfine lattices (green crosses). Lines are drawn to guide the eye.
quark ( $6.280(10) \mathrm{GeV}$ [18]). We agree, within $2 \sigma$ with both results even allowing for the fact that the comparison within lattice QCD can be done before any shifts are made or errors allowed for them. This is a strong confirmation of the control over errors that we now have in lattice QCD.

The method given here for determining $m_{B_{c}}$ (as for the method for $m_{B_{s}}$ in section III B) does depend on the experimental $\eta_{b}$ mass; the mass difference determined in lattice QCD is not particularly sensitive to it but when the mass is reconstructed from the difference, $m_{\eta_{b}} / 2$ is added in. Recent results from the Belle collaboration [29] have $M_{\eta_{b}}=9.402(2) \mathrm{GeV}$, significantly higher than the previous world-average [17]. Using the Belle result for $M_{\eta_{b}}$ pushes our values for $m_{B_{c}}$ and $m_{B_{s}} 6 \mathrm{MeV}$ higher. In both cases this improves the agreement with experiment but is not significant given the 11 MeV error. Note that our earlier NRQCD results are hardly affected at all by a change in the $\eta_{b}$ mass because they determined a mass difference to the spin-average of the $\Upsilon$ and $\eta_{b}$ masses, which is dominated by the $\Upsilon$ mass.

Results for the $H_{c}$ decay constant, $f_{H_{c}}$, are also given in Table VII. The rate for $B_{c}$ leptonic decay to $l \nu$ via a $W$ boson is proportional to the square of the decay constant multiplied by CKM element $V_{c b}$ as in eq. (4). In practice this decay will be very hard to see experimentally, but a lattice QCD calculation of the decay constant also provides a useful test for phenomenological model calculations.

The results at different values of $m_{c}$ can again be used to tune the decay constant accurately to the result at the physical $c$ quark mass. Figure 6 shows the dependence of $f_{H_{c}}$ on $M_{\eta_{c}}$ acting as a proxy for the $c$ quark mass. Results on fine and superfine lattices are shown - there is clear agreement on the physical slope of $f_{H_{c}}$ with $M_{\eta_{c}}$ between superfine and fine and it does not vary with the heavy quark mass. The slope is small, approximately 0.06 , but clearly visible. We will compare this to the


FIG. 7: Results for the heavy-charm decay constant plotted as a function of the pseudoscalar heavyonium mass. Results for coarse, fine, superfine and ultrafine lattices appear from left to right. The lattice QCD results have been adjusted for slight mistuning of the $c$ quark mass. The colored dashed lines give the fitted function for that lattice spacing. The black line with grey error band gives the physical curve derived from our fit.
slope for $f_{H_{s}}$ with $m_{s}$ in section IV.
The $H_{c}$ decay constant is plotted as a function of $M_{\eta_{h}}$ in Figure 7. Notice that it is much flatter than the corresponding plot for $f_{\eta_{h}}$ (Figure 1). We expect behaviour as $1 / \sqrt{M_{\eta_{h}}}$ whether we view heavy-charm as a heavylight system (in which case the behaviour will be similar to heavy-strange) or as a heavy-heavy system (in which case the argument becomes that $\psi(0)$ depends on the reduced mass $\mu$, tending to $m_{c}$ for large $m_{h}$, and then the decay constant falls as the square root of the heavy mass).

As before, we fit $f_{H_{c}}$ to the function of $M_{\eta_{h}}$ (above 4 GeV ) described in section II. We take the leading term given in Table III to be that expected from HQET arguments appropriate to heavy-light physics. Our fit has $\chi^{2}=0.7$ for 11 degrees of freedom and gives result:

$$
\begin{equation*}
f_{B_{c}}=0.427(6)(2) \mathrm{GeV} \tag{16}
\end{equation*}
$$

Here the first error is from the fit and the second from additional systematic effects missing from our lattice QCD calculation. These we estimate based on the arguments given for the $\eta_{h}$ in section III A. The error from missing electromagnetism and from sea quark mass effects we take to be the same as for the $\eta_{b}$ at $0.4 \%$ and $0.1 \%$ respectively; missing $c$ in the sea should be a factor of $m_{c} / m_{b}$ smaller at $0.04 \%$. Table VIII gives the complete error budget.
$f_{B_{c}}$ can be converted into a branching fraction for leptonic decay using the formula of eq. (4) and the unitarity value of $V_{c b}$. We predict a branching fraction to $\tau \nu$ of $0.0194(18)$. The error here comes mainly from the experimental determination of the $B_{c}$ lifetime with a smaller effect from the uncertainty in $V_{c b}$. Our value for $f_{B_{c}}$ contributes a $3 \%$ error. Because of helicity suppression the
branching fraction smaller for other lepton final states ( $8 \times 10^{-5}$ to $\mu \nu$, for example).

The value we obtain for $f_{B_{c}}$ can be compared to results from potential models. As discussed earlier in the context of $f_{\eta_{h}}$, potential model results have a lot of variability and raw values for $\psi(0)$ need renormalisation. A more useful comparison is to compare ratios. Our lattice QCD results give $f_{B_{c}} / f_{\eta_{c}}=1.08(1)$ and $f_{\eta_{h}} / f_{B_{c}}=1.57(2)$. The range of potentials considered in [22] give values from 0.90 to 1.02 for $f_{B_{c}} / f_{\eta_{c}}$ and 1.34 to 1.72 for $f_{\eta_{h}} / f_{B_{c}}$. Again the largest number is always from the Cornell potential. Potential model values for $\psi(0)$ converted to $f_{B_{c}}$ simply using $f=\psi(0) \sqrt{12 / M_{B_{c}}}$ yield results varying from 0.5 to 0.7 GeV i.e. significantly larger than the well-defined value for $f_{B_{c}}$ from lattice QCD .

The values for $f_{B_{c}}$ from potential models provide input to estimates of the production cross-section of the $B_{c}$ at the LHC. In the factorisation approach the cross-section is proportional to the square of $f_{B_{c}}$, with typical values for $f_{B_{c}}$ being taken as 0.48 GeV 30 . Our results indicate that this could be leading to a $25 \%$ overestimate of the production rate.

## IV. DISCUSSION

An interesting issue is to what extent the $B_{c}$ meson is a heavy-heavy particle and to what extent, a heavylight one at the physical values we have for $b$ and $c$ quark masses. Here we address this by comparing the behaviour of $B_{c}$ properties to those of $\eta_{h}$ and $B_{s}$ using the results from section III.

An alternative to calculating $\Delta_{H_{c}, h h}$ to study the heavy-charm meson mass is to take differences between heavy-charm and heavy-strange and charmstrange mesons. We define

$$
\begin{equation*}
\Delta_{H_{c}, h s}=M_{H_{s}}+M_{D_{s}}-M_{H_{c}} \tag{17}
\end{equation*}
$$

so that $\Delta_{H_{c}, h s}$ is a positive quantity. Once again it amounts to a difference in binding energies but now between a set of mesons that are all effectively 'heavy-light' states. Indeed a study of $\Delta_{H_{c}, h s}$ shows us to what extent the $B_{c}$ can be considered a heavy-light particle rather than, or as well as, a heavy-heavy one.

Figure 8 shows $\Delta_{H_{c}, h s}$, with all results tuned accurately to the correct $c$ and $s$ masses, as a function of the heavy quark mass, again given by the $\eta_{h}$ mass. In fact $\Delta_{H_{c}, h s}$ shows very little dependence on the heavy quark mass above a value of $M_{\eta_{h}}$ of about 6 GeV . HQET would expect the leading $m_{h}$-dependent piece of $\Delta_{B_{c}, h s}$ to be given by the difference of the expectation values of the kinetic energy operator, $p_{h}^{2} / 2 m_{h}$, for the heavy quark in a heavy-charm meson and a heavy-strange meson, ignoring the effect of spin-dependent terms which are expected to be smaller. Figure 8 shows that this difference is not large i.e. the charm quark is behaving in a similar way to a light quark (but does have a larger expectation value for its kinetic energy operator as might be expected) when
combined with a heavy quark of order twice its mass or heavier.

We fit $m_{H_{c}, h s}$ as described in section IT and using the fit form and priors tabulated in Table III. Our fit has $\chi^{2}$ of 0.3 for 14 degrees of freedom. It returns the coefficient of the first term in $M_{\eta_{h}}^{-1}$ as $-0.4(8) \mathrm{GeV} / M_{\eta_{h}}$. This quantifies the statement made above about the slope of $1 / m_{h}$ corrections. The coefficient is not very accurately determined because we allow for many higher order terms. In fact the sign of the slope is clear from Figure 8 with a positive slope with $M_{\eta_{h}}$ corresponding to a negative value for the coefficient of the $1 / M$ term, as expected.

The variation of $\Delta_{H_{c}, h s}$ with $M_{\eta_{c}}$ agrees well with that found in our calculation using NRQCD $b$ quarks [18] giving a slope of 0.07 at the $b$. Likewise the variation with $M_{\eta_{s}}^{2}$ also agrees well with the slope of 0.4 found in [18].

Our fit to $\Delta H_{c}, h s$ is independent of our earlier fit to $\Delta_{H_{c}, h h}$ (although it uses some of the same numbers) and so the results provide a consistency check. We find at $h=b$ that:

$$
\begin{equation*}
\Delta_{B_{c}, b s}=1.052(9)(3) \mathrm{GeV} \tag{18}
\end{equation*}
$$

which agrees well within $1 \sigma$ with the same quantity calculated using NRQCD $b$ quarks [18. The result when $h=c$ is consistent within $1 \sigma$ with double the result from $m_{D_{s}}-m_{\eta_{c}} / 2$ given in [10]. The first error above is from the fit and the second from the systematic error for sea quark mass effects, taking the same 1 MeV as for $\Delta_{B_{c}, b b}$, and the effects of missing electromagnetism and $c$ in the sea. The shifts and errors for these latter effects are given in Table III and we take those errors to be correlated. The value above for $\Delta_{B_{c}, b s}$ combined with experimental results for $M_{B_{s}}$ and $M_{D_{s}}$ [17] (the net shift from Table II amounts to a negligible 0.2 MeV ) gives:

$$
\begin{equation*}
M_{B_{c}}=6.285(9)(3) \mathrm{GeV}, \tag{19}
\end{equation*}
$$

consistent within $2 \sigma$ with our result from $\Delta_{B_{c}, b b}$ given in section III, and slightly more accurate. We therefore adopt it as our final result here. The complete error budget for $\Delta_{B_{s}, b s}$ is given in Table VIII.

In figure 9 we show the ratio of $\eta_{h}$ and $H_{c}$ decay constants to that of the $H_{s}$, plotted from our physical curves as a function of $M_{\eta_{h}}$. The ratio $f_{\eta_{h}} / f_{H_{s}}$ rises strongly with $M_{\eta_{h}}$, because of the big difference in the dynamics of heavy-heavy and heavy-strange mesons, whereas the ratio $f_{H_{c}} / f_{H_{s}}$ tends to a constant at large $M_{\eta_{h}}$. As explained in section IIIC this latter behaviour would be expected whether the heavy-charm is viewed as a heavyheavy or heavy-light state, because the reduced mass of the heavy-charm system is controlled by the charm mass in the large heavy mass limit.

Further insight comes from comparing the dependence of the heavy-charm and heavy-strange decay constants on $m_{c}$ and $m_{s}$ respectively. Figure 10 plots the relative change of $f_{H_{c}}$ or $f_{H_{s}}$ to its value at the tuned mass point for a given relative change in the light quark mass. The strange quark mass is monitored by the value of $M_{\eta_{s}}^{2}$,


FIG. 8: Results for the mass difference between the heavycharm meson and the corresponding heavy-strange and charm-strange mesons plotted as a function of the pseudoscalar heavyonium mass. Results for coarse, fine, superfine and ultrafine lattices appear from left to right. The lattice QCD results have been adjusted for slight mistuning of the $c$ and $s$ quark masses. The colored dashed lines give the fitted function for that lattice spacing. The black line with grey error band gives the physical curve derived from our fit. The black circles with error bars at $M_{\eta_{b}}$ and $M_{\eta_{c}}$ give experimental values adjusted for the effects from electromagnetism, $\eta_{b} / \eta_{c}$ annihilation and $c$ quarks in the sea, none of which is included in the lattice QCD calculation.


FIG. 9: Results for the ratio of pseudoscalar decay constants, heavy-charm and heavy-heavy to heavy-strange plotted as a function of the pseudoscalar heavyonium mass. The results are obtained from the physical curves given in Figures 1, 3 and 7 .
the charm mass by $M_{\eta_{c}}$. The results come from the fine lattices, set 3 , where we have multiple $m_{c}$ and $m_{s}$ values close to the tuned point. Results are plotted for two values of the heavy quark mass, $m_{h} a=0.7$ and $m_{h} a=$ 0.85 but little difference between them is seen.

The dependence of $f_{H_{s}}$ on $m_{s}$ is not very strong [4, as expected since $f_{H_{s}}$ and $f_{H}$ differ only by around $20 \%$ for a change by a factor of 27 in light quark mass. The dependence of $f_{H_{c}}$ on $m_{c}$ is larger by about a factor of


FIG. 10: Comparison of the effect of 'detuning' the charm and strange quark masses on the heavy-charm and heavy-strange decay constants. Open squares show the fractional change in $f_{H_{c}}$ for a given fractional change in $M_{\eta_{c}}$ (as proxy for $m_{c}$ ) for two different heavy quark masses (in blue $m_{h} a=0.7$ and red $m_{h} a=0.85$ ) on the fine lattices set 3. Burst show the fractional change in $f_{H_{s}}$ for a given fractional change in $M_{\eta_{s}}^{2}$ (as proxy for $m_{s}$ ) for the same two heavy quark masses on set 3. Lines are drawn to guide the eye.

| $M_{\eta_{h}}$ | $f_{\eta_{h}}$ | $f_{H_{s}}$ | $f_{H_{c}}$ | $\Delta_{H_{s}, h h}$ | $\Delta_{H_{c}, h h}$ | $\Delta_{H_{c}, h s}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3 | $0.394(2)$ | $0.249(2)$ | - | $0.477(2)$ | $0.000(0)$ | $0.956(6)$ |
| 4 | $0.452(2)$ | $0.251(2)$ | $0.417(6)$ | $0.520(3)$ | $0.004(1)$ | $0.994(7)$ |
| 5 | $0.501(3)$ | $0.249(2)$ | $0.427(3)$ | $0.554(4)$ | $0.015(1)$ | $1.014(6)$ |
| 6 | $0.546(4)$ | $0.244(3)$ | $0.434(4)$ | $0.581(6)$ | $0.027(2)$ | $1.028(6)$ |
| 7 | $0.586(4)$ | $0.237(3)$ | $0.435(4)$ | $0.605(7)$ | $0.039(3)$ | $1.038(7)$ |
| 8 | $0.623(5)$ | $0.231(4)$ | $0.433(5)$ | $0.626(9)$ | $0.050(5)$ | $1.045(8)$ |
| 9 | $0.655(6)$ | $0.224(4)$ | $0.429(6)$ | $0.645(11)$ | $0.061(8)$ | $1.050(8)$ |

TABLE IX: Values for the various quantities that we fit here evaluated at masses, $M_{\eta_{h}}$, between that of $c$ and $b$. These are obtained from our fit functions at $a=0$ and tuned $s$ and $c$ masses. All numbers are in GeV . There is no result for $f_{H_{c}}$ at 3 GeV because that point is not included in that fit.
two. However the slope of the Figure 10 is $1 / 3$ (see also Figure 6), much less than the slope of 1 expected if $f_{B_{c}} \propto$ $m_{c}$. This latter behaviour would be approximately that expected in a heavy-heavy picture in which $\psi(0) \propto \mu$, with the reduced mass, $\mu$, close to $m_{c}$ in the $B_{c}$ case. The linear behaviour of $\psi(0)$ would be consistent with the picture we have of the $\eta_{h}$ in Figure 1, where $\mu \approx M_{\eta_{h}} / 4$, using $b \approx 0.5$.

## V. CONCLUSIONS

By using a relativistic approach to heavy quarks (HISQ) which has relatively small discretisation errors we have been able to map out the dependence on heavy quark mass of the pseudoscalar heavyonium, heavystrange and heavy-charm decay constants and the heavystrange and heavy-charm meson masses, complementing results in [3, 4].

We find the heavyonium decay constant surprisingly


FIG. 11: Summary of heavy quark mass dependence of decay constants for the pseudoscalar $H_{c}, H_{s}$ and $\eta_{h}$ mesons. The grey bands show our physical curves from Figures 1, 3 and 7.
close in value to the experimental results for the charmonium and bottomonium vector decay constants. Work is underway to confirm this result using NRQCD for the heavy quark and to establish accurate results for the corresponding vector decay constants in lattice QCD. Although the $\eta_{h}$ decay constant has no simple connection to an observed experimental rate, it is useful for comparison and calibration of lattice QCD calculations in heavy quark physics since it can be determined to $1 \%$, as we have done here.

Our result for the $B_{c}$ meson mass agrees well using the two different mass splittings, $\Delta_{B_{c}, h h}$ and $\Delta_{B_{c}, h s}$ and also agrees with the experimental value. This is confirmation of our earlier result [18] using NRQCD $b$ quarks and HISQ light quarks.

We determine the $B_{c}$ decay constant as $427(6) \mathrm{MeV}$, for the first time in full QCD , predicting a leptonic branching ratio for the $B_{c}$ to $\tau \nu$ of $1.9(2) \%$ (where the uncertainty comes from $t_{B_{c}}$, not $f_{B_{c}}$ ). Our result for $f_{B_{c}}$ is significantly smaller than that from some potential model calculations, including those being used to estimate LHC production cross-sections 30. The best way to determine the $B_{c}$ leptonic decay rate, and hence $f_{B_{c}}$, from experiment may be using a high luminosity $e^{+} e^{-}$ collider operating at the $Z$ peak [36, 37].

By mapping out the dependence on the heavy quark mass of the $H_{c}, H_{s}$ and $\eta_{h}$ decay constants we are able to see the differences between the three systems. This is summarised in Figure 11 where we give the physical curves determined from our fits. In section IV we provide evidence that the $B_{c}$ behaves, at least in some ways, more like a heavy-light system than a heavy-heavy one. We previously noticed this effect in [38] when finding that the mass difference between $B_{c}^{*}$ and $B_{c}$ was very close to the difference between $B_{s}^{*}$ and $B_{s}$.

Table IX gives results extracted from our fits at intermediate values of $M_{\eta_{h}}$ from $M_{\eta_{c}}$ to $M_{\eta_{b}}$ for com-
parison to future lattice QCD calculations or to phenomenological models. The values are determined by evaluating our fit function in the continuum limit and at tuned $s$ and $c$ masses, corresponding to the black line in Figs. 1, 2, 3, 4, 7 and 8.

In Figure 12 we summarise the current picture for the decay constants of gold-plated mesons, determined from lattice QCD and from experiment. For lattice QCD we use the best existing results which dominate the world averages [1, 4, 10, 11, 31, 32]. For the experimental values for the unflavored vectors we use leptonic widths to $e^{+} e^{-}$from the Particle Data Tables 17 and eq. 10 . For the flavored pseudoscalars the determination of the decay constant from experiment requires the input of a value for the associated CKM element, for example from the unitarity fit to the CKM matrix [17. We update the $D$ and $D_{s}$ experimental determinations to the averages including new results from BESIII [34] and Belle [35] respectively.

This plot goes beyond the traditional plot of the mass spectrum [1] to look at a number which is related to the internal structure of the meson. The energy scale for decay constants is controlled by internal momenta inside the meson and so is much compressed over the scale for masses (which covers a large range simply because quark masses have a large range). The pseudoscalar meson decay constants are well filled in but more work is needed to obtain the vector decay constants to the same level of accuracy. This is underway and once complete, this plot will provide a very stringent test of QCD that would be impossible with any method other than lattice QCD.

From our results here and in [3, 4] we see that the relativistic heavy quark approach using the HISQ formalism can successfully give results for the $b$ quark. Future work will use even finer lattices. For $a=0.03 \mathrm{fm}$, for example, the $b$ quark mass in lattice units is around 0.5 and so we can easily achieve this mass without the need for extrapolation.

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FIG. 12: Spectrum of the decay constants of gold-plated particles from experiment (using values for CKM elements where needed) and from lattice QCD. Lattice QCD results are divided into postdictions (green open squares) and predictions (blue open circles). Results for $f_{B_{c}}$ and $f_{\eta_{b}}$ come from this paper, $f_{D_{s}}$ and $f_{\eta_{c}}$ from [10, $f_{\pi}$ and $f_{K}$ from [31, $f_{B}$ from 11 and $f_{D}$ from [32. Experimental results are given by red shaded bars. For unflavored vector mesons these come from [17] using eq. 10. $f_{\pi}$ and $f_{K}$ are from [17, 33, $f_{D}$ is the updated experimental average from 34] and $f_{D_{s}}$, from [35]. $f_{B}$ is not well-determined from experiment. We use the result from (1) using averages from 17.
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# Precision tests of the $J / \psi$ from full lattice QCD: mass, leptonic width and radiative decay rate to $\eta_{c}$ 

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#### Abstract

We calculate the $J / \psi$ mass, leptonic width and radiative decay rate to $\gamma \eta_{c}$ from lattice QCD including $u, d$ and $s$ quarks in the sea for the first time. We use the Highly Improved Staggered Quark formalism and nonperturbatively normalised vector currents for the leptonic and radiative decay rates. Our results are: $M_{J / \psi}-M_{\eta_{c}}=116.5(3.2) \mathrm{MeV} ; \Gamma\left(J / \psi \rightarrow e^{+} e^{-}\right)=5.48(16) \mathrm{keV}$; $\Gamma\left(J / \psi \rightarrow \gamma \eta_{c}\right)=2.49(19) \mathrm{keV}$. The first two are in good agreement with experiment, with $\Gamma(J / \psi \rightarrow$ $e^{+} e^{-}$) providing a test of a decay matrix element in QCD, independent of CKM uncertainties, to $2 \%$. At the same time results for the time moments of the correlation function can be compared to values from the charm contribution to $\sigma\left(e^{+} e^{-} \rightarrow\right.$ hadrons $)$, giving a $1.5 \%$ test of QCD. Our results show that an improved experimental error would enable a similarly strong test from $\Gamma\left(J / \psi \rightarrow \gamma \eta_{c}\right)$.


## I. INTRODUCTION

Precision tests of lattice QCD against experiment are critical to provide benchmarks against which to calibrate the reliability of predictions from lattice QCD [1]. Most tests to date have relied on the spectrum of gold-plated hadron masses - for example, the mass of the $D_{s}$ meson can be calculated in lattice QCD with an error of 3 MeV (having fixed the masses of the $c$ and $s$ masses from other mesons) and the result agrees with experiment [2, 3]. Here we give another such test by determining the mass of the $J / \psi$ to a precision of 3 MeV .

Tests of decay matrix elements are harder to do very accurately. We need precision tests of these because it is the predictions of decay matrix elements from lattice QCD that enable, for example, progress with the flavor physics programme [4] of over-determining the CKM matrix to find signs of new physics [5]. The leptonic decay rate of the $\pi$ via a $W$ boson provides one such test. The QCD input to this is the pion decay constant, which is determined to $1 \%$ in lattice QCD [6]. If we take $V_{u d}$ from nuclear $\beta$ decay [7], we have a $2 \%$ determination of the leptonic decay rate to be compared to experiment. The leptonic decay rates of other charged pseudoscalars can also be determined to a few percent from lattice QCD 4 but then the comparison with experiment is generally needed to determine the appropriate CKM element. Independent tests of matrix elements, without CKM uncertainties, come only from electromagnetic decays. Here we provide two such tests through two different decay rates

[^300]of the $J / \psi$ : annihilation to $e^{+} e^{-}$via a photon and radiative decay to the $\eta_{c}$. We give the first results from full lattice QCD including $u, d$ and $s$ quarks in the sea, although earlier calculations have been done in quenched QCD [8] and including $u$ and $d$ sea quarks [9, 10].

We are able to determine these matrix elements to a few percent because of our development of an accurate and fully relativistic approach to $c$ quarks (as well as $u, d$ and $s$ ) in lattice QCD called the Highly Improved Staggered Quark (HISQ) formalism [11]. In this formalism we are able to normalise the vector current which mediates the electromagnetic decay accurately and nonperturbatively and we show how to do that here.

The layout of the paper is as follows: section III describes the lattice calculation and then section III gives results for the $J / \psi$ mass, leptonic width (along with time moments of the $J / \psi$ correlator) and radiative decay rate in turn. We compare our results to experiment and to previous lattice QCD calculations in section IV. Section $\square$ gives our conclusions. The Appendices discuss the more technical issues of discretisation errors and our two different methods for current renormalisation.

## II. LATTICE CALCULATION

We use 6 ensembles of lattice gluon configurations at 4 different, widely separated, values of the lattice spacing, provided by the MILC collaboration [12]. The configurations include the effect of $u, d$ and $s$ quarks in the sea with the improved staggered (asqtad) formalism. The $u$ and $d$ masses are taken to be the same with $m_{u / d} / m_{s}$ approximately 0.2 on most of the ensembles. Based on our experience of other gold-plated mesons [2] we expect sea quark mass effects to be small for the $J / \psi$ because it

| Set | $r_{1} / a$ | $a u_{0} m_{l}^{a s q}$ | $a u_{0} m_{s}^{a s q}$ | $L_{s} / a$ | $L_{t} / a$ | $\delta x_{l}$ | $\delta x_{s}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | $2.647(3)$ | 0.005 | 0.05 | 24 | 64 | 0.11 | 0.43 |
| 2 | $2.618(3)$ | 0.01 | 0.05 | 20 | 64 | 0.25 | 0.43 |
| 3 | $2.658(3)$ | 0.01 | 0.03 | 20 | 64 | 0.25 | -0.14 |
| 4 | $3.699(3)$ | 0.0062 | 0.031 | 28 | 96 | 0.20 | 0.19 |
| 5 | $5.296(7)$ | 0.0036 | 0.018 | 48 | 144 | 0.16 | -0.03 |
| 6 | $7.115(20)$ | 0.0028 | 0.014 | 64 | 192 | 0.17 | 0.04 |

TABLE I: Ensembles (sets) of MILC configurations used for this analysis. The sea asqtad quark masses $m_{l}^{\text {asq }}(l=u / d)$ and $m_{s}^{a s q}$ are given in the MILC convention where $u_{0}$ is the plaquette tadpole parameter. The lattice spacing values in units of $r_{1}$ after 'smoothing' are given in the second column [12. Here sets 1, 2 and 3 are 'coarse'; set 4, 'fine'; set 5 'superfine' and set 6 'ultrafine'. The size of the lattices is given by $L_{s}^{3} \times L_{t}$. The final two columns give the difference between the sea quark mass and its physical value in units of the $s$ quark mass [2].
has no valence light quarks. We can test this by comparison of results on sets 1 and 2 where the sea value of $m_{u, d}$ changes by a factor of two and with set 3 where the sea value of $m_{s}$ changes by $70 \%$. Table $\mathbb{\square}$ lists the parameters of the ensembles.

The lattice spacing is determined on an ensemble-byensemble basis using a parameter $r_{1}$ that comes from fits to the static quark potential calculated on the lattice 12 . This parameter has small statistical/fitting errors but its physical value is not accessible to experiment and so must be determined using other quantities, calculated on the lattice, that are. We have determined $r_{1}=0.3133(23) \mathrm{fm}$ using four different quantities ranging from the ( $2 \mathrm{~S}-1 \mathrm{~S}$ ) splitting in the $\Upsilon$ system to the decay constant of the $\eta_{s}$ (fixing $f_{K}$ and $f_{\pi}$ from experiment) [13]. Using our value for $r_{1}$ and the MILC values for $r_{1} / a$ given in Table I we can determine $a$ in fm on each ensemble or, equivalently, $a^{-1}$ in GeV needed to convert lattice quantities to physical units.

On these ensembles we calculate $c$ quark propagators using the HISQ action and combine them into meson correlation functions. The quark propagators are made from a 'random wall' source - a color 3-vector of $\mathrm{U}(1)$ random numbers - on a given timeslice to reduce the statistical noise. An added reduction comes from the use of a random starting point for the equally spaced time-sources we use on the coarse and fine ensembles. We include only connected correlation functions here disconnected contributions for the $J / \psi$ are related to its hadronic width which is in keV and therefore negligible here.

The $c$ quark mass is tuned from the $\eta_{c}$ meson mass [2]. The appropriate 'experimental' mass for the $\eta_{c}$ for our calculations is $2.986(3) \mathrm{GeV}$, differing from the experimental result of $2.981(1) \mathrm{GeV}$ [7] because of missing electromagnetic, $\eta_{c}$ annihilation and $c$-in-the-sea effects that we estimate perturbatively [14]. The HISQ lattice $c$ quark masses for the ensembles we are using were determined in [2].

Meson masses and decay constants are determined from simple ' 2 -point' meson correlation functions made from combining quark propagators with appropriate spin matrices at source and sink to project onto the correct $J^{P C}$. For staggered quarks, where the spin degree of freedom has disappeared, the spin projection matrices are replaced with space-time-dependent phases of $\pm 1$. Because of fermion-doubling, there are in fact 16 'tastes' of every meson made by combining a point-splitting of the quark and antiquark source and sink along with the appropriate $\pm 1$ phases. The most accurate meson correlation functions come from either local or 1-link separated sources and sinks and we will restrict ourselves to these here. Because the taste-splittings are discretisation effects we are free to use whichever taste is the most convenient for a given calculation.

For the pseudoscalar mesons the mass differences between the different tastes have a simple picture with the mass increasing as the amount of point-splitting in the source/sink operator increases. The lightest mass particle is the Goldstone meson whose correlator is simply the modulus squared of the propagator and whose squared mass vanishes linearly with the quark mass. This is the one that is used to tune the quark mass. The other taste pseudoscalar mesons have a mass for which the difference of mass-squared with the Goldstone meson is a constant with quark mass which vanishes as $\alpha_{s}^{2} a^{2}$. These tastesplitting discretisation errors are particularly small with the HISQ action [11]. They also become smaller, in proportion to the meson mass, as the meson mass increases and so are very small for mesons made of $c$ quarks [11]. The mass difference between the Goldstone meson and the next heaviest pseudoscalar meson is visible, however. Both masses can be determined very accurately in lattice QCD because they both correspond to local operators. The Goldstone meson corresponds to the local $\gamma_{5}$ operator and the local non-Goldstone to the local $\gamma_{0} \gamma_{5}$ operator. We will use both of these mesons in our calculation of the radiative decay rate of the $J / \psi$.

Vector meson taste-splittings are significantly smaller than for pseudoscalars and typically not visible for light mesons above the statistical errors. For the charmonium vectors we use the local $\gamma_{i}$ operator to determine the leptonic decay rate and two different 1-link split operators for the radiative decay. We discuss mass differences from taste-splittings further in Appendix A.

## III. RESULTS

$$
\text { A. } M_{J / \psi}
$$

The determination of the mass of the $J / \psi$ is most accurately done through the determination of the charmonium hyperfine splitting, i.e. the mass difference with the pseudoscalar $\eta_{c}$ meson. For the $\eta_{c}$ we use the Goldstone meson, as discussed in section II, because this is the most accurately determined in lattice QCD and is the meson
we use to fix the $c$ quark mass. We studied this meson in detail in [2]. For the $J / \psi$ we use the local $\gamma_{i}$ operator to create and destroy the vector meson. The $J / \psi$ correlators are then obtained by combining quark propagators from the default random wall with antiquark propagators from a source using the same random wall but patterned with phases, for example $(-1)^{x}$ for the vector polarised in the $x$ direction. $(-1)^{x}$ is also inserted at the sink where the propagators are tied together.

The $J / \psi$ and $\eta_{c}$ correlators at zero spatial momentum are fit simultaneously so that correlations between them are taken into account. The fit form for the average $J / \psi$ correlator as a function of time separation between source and sink, $t$, is:

$$
\begin{equation*}
\bar{C}_{2 p t}(t)=\sum_{i_{n}, i_{o}} a_{i_{n}}^{2} \mathrm{fn}\left(M_{i_{n}}, t\right)-\tilde{a}_{i_{o}}^{2} \mathrm{fo}\left(\tilde{M}_{i_{o}}, t\right) \tag{1}
\end{equation*}
$$

with

$$
\begin{align*}
\operatorname{fn}(M, t) & =e^{-M t}+e^{-M\left(L_{t}-t\right)} \\
\operatorname{fo}(M, t) & =(-1)^{t / a} \operatorname{fn}(M, t) \tag{2}
\end{align*}
$$

and $L_{t}$ the time extent of the lattice. $i_{n}=0$ is the ground state and larger $i_{n}$ values denote radial or other excitations with the same $J^{P C}$ quantum numbers. The $M_{i_{n}}$ are the masses of the corresponding particles. There are 'oscillating' terms coming from opposite parity states, denoted $i_{o}$. The Goldstone $\eta_{c}$ meson has the same fit form except that there are no oscillating contributions (when the $\eta_{c}$ is at rest). Note that we do not use any 'smearing' functions for the propagators at either source or sink.

To fit we use a number of exponentials $i_{n}$, and where appropriate $i_{o}$, in the range $2-6$, loosely constraining the higher order exponentials by the use of Bayesian priors [15]. As the number of exponentials increases, we see the $\chi^{2}$ value fall below 1 and the results for the fitted values and errors for the parameters for the ground state $i=0$ stabilise. This allows us to determine the ground state parameters $a_{0}$ and $M_{0}$ as accurately as possible whilst including the full systematic error from the presence of higher excitations in the correlation function. We take the fit parameters to be the logarithm of the ground state masses $M_{0}$ and $\tilde{M}_{0}$ and the logarithms of the differences in mass between successive radial excitations (which are then forced to be positive). The Bayesian prior value for $M_{0}$ for the $\eta_{c}$ is obtained from a simple 'effective mass' in the correlator and the prior width on the value is taken as 0.3 . The prior value on $M_{0}$ for the $J / \psi$ is taken to be $100 \pm 50 \mathrm{MeV}$ above the $\eta_{c}$. The prior value for mass splittings to and between excitations is taken as $600(300) \mathrm{MeV}$. The amplitudes $a_{i_{n}}$ and $a_{i_{o}}$ are given prior widths of 1.0 . We apply a cut on the range of eigenvalues from the correlation matrix that are used in the fit of $10^{-4}$. We also cut out small $t / a$ (and $\left.\left(L_{t}-t\right) / a\right)$ values below 6 from our fit to reduce the effect of higher excitations.


FIG. 1: Our average $J / \psi$ correlator divided by the ground state exponential ( $\mathrm{fn}\left(M_{0}, t\right)$ from eq. 2 Z ) as a function of lattice time. Lines are drawn to join the points (which include statistical errors) for clarity. The fitted result for the ground state amplitude, $a_{0}^{2}$, is given by the blue band. The fit includes 6 normal exponentials and 6 oscillating ones, which are responsible for the oscillating behaviour clearly seen in the results.

Figure 1 shows the quality of our results with a plot of the $J / \psi$ correlation function. It is divided by the groundstate exponential function so that it shows a plateau in the centre of value $a_{0}^{2}$. The results for the ground-state masses in lattice units of the $J / \psi$ and $\eta_{c}$ and the difference between them, $a \Delta M_{h y p}$, are given in Table II. The difference is typically more accurate than that obtained by simply subtracting the masses because of the correlation between the correlators.

The hyperfine splitting is converted to physical units using the values for $a$ on each ensemble as discussed in section III The results are shown in Figure 2. Figure 2 includes the error from the determination of the lattice spacing on each point. This dominates the error but is correlated between the points and that should be borne in mind in looking at the figure. It is important to realise that the naive lattice spacing error is magnified by a factor of approximately two in the hyperfine splitting because of the inverse relationship between hyperfine splitting and quark mass. For example, a shift by uncertainty $\delta$ upwards in the inverse lattice spacing causes a shift upwards in the meson mass by the same proportion. To determine the total effect of this on the hyperfine splitting we must include the effect of retuning the $c$ quark mass to make the meson mass correct again. This means in this case retuning the quark mass down by fraction $\delta$ which shifts the hyperfine splitting upward by a further factor of $\delta$ to that coming simply from the lattice spacing change. Thus the change in the hyperfine splitting, rep-

| Set $N_{\text {cfg }} \times N_{t}$ | $m_{c} a$ | $\epsilon$ | $a M_{\eta_{c}}$ | $a M_{J / \psi}$ | $a \Delta M_{h y p}$ | $a f_{J / \psi} / Z$ | $Z_{c c}$ |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | $2099 \times 8$ | 0.622 | -0.221 | $1.79118(4)$ | $1.85934(8)$ | $0.06817(6)$ | $0.2810(2)$ | $0.979(12)$ |
| 2 | $2259 \times 4$ | 0.63 | -0.226 | $1.80851(5)$ | $1.87797(10)$ | $0.06946(8)$ | $0.2855(2)$ | $0.979(12)$ |
| 2 | $2259 \times 8$ | 0.66 | -0.244 | $1.86667(4)$ | $1.93430(9)$ | $0.06763(7)$ | $0.2925(2)$ | $0.974(12)$ |
| 3 | $323 \times 8$ | 0.617 | -0.218 | $1.78212(12)$ | $1.85081(23)$ | $0.06869(17)$ | $0.2804(5)$ | $0.979(12)$ |
| 4 | $566 \times 4$ | 0.413 | -0.107 | $1.28052(7)$ | $1.32901(12)$ | $0.04849(10)$ | $0.1829(2)$ | $0.983(12)$ |
| 5 | $200 \times 2$ | 0.273 | -0.0487 | $0.89948(8)$ | $0.93369(13)$ | $0.03421(11)$ | $0.1244(3)$ | $0.986(12)$ |
| 6 | $208 \times 1$ | 0.193 | -0.0247 | $0.66649(6)$ | $0.69217(11)$ | $0.02568(10)$ | $0.0925(3)$ | $0.990(12)$ |

TABLE II: Results in lattice units for the masses of $\eta_{c}$ and $J / \psi$ and their difference on each ensemble along with the raw (unrenormalised) decay constant and $Z$ factor for the $J / \psi$. Columns 3 and 4 give the bare HISQ charm quark mass, tuned from the $\eta_{c}$ and the corresponding coefficient $\epsilon$ used in the Naik discretization improvement term of the HISQ action [2]. All of the charm quark masses are very well tuned except for the lower result on set 2 ( $m_{c} a=0.66$ ), which was deliberately mistuned to assess the sensitivity of quantities to the tuning. Of the remaining masses the least well-tuned is on superfine set 5 where $M_{\eta_{c}}$ is $0.5 \%$ too high. Column 2 gives the number of configurations used and the number of time sources for propagators on each configuration. Results are binned on time sources and binned over neighbouring configurations for sets 5 and 6 . The $J / \psi$ correlators are averaged over polarisations except on sets 2 and 3 where only one polarisation was calculated. The results for the $\eta_{c}$ masses are also given in [2]. They differ slightly from these in some cases because of fitting simultaneously with $J / \psi$ correlators. The $Z$ factors are taken from moment 4 of the nonperturbative (on the lattice) current-current correlator method described in Appendix B1.


FIG. 2: Results for the charmonium hyperfine splitting plotted as a function of lattice spacing. For the $x$-axis we use $\left(m_{c} a\right)^{2}$ to allow the $a$-dependence of our fit function (eq. (3)) (blue dashed line with grey error band) to be displayed simply. The data points have been corrected for $c$ quark mass mistuning and sea quark mass effects, but the corrections are smaller than the error bars. We do not include on the plot the deliberately mistuned $c$ mass but it is included in the fit to constrain the $c$ mass dependence. The errors shown include (and are dominated by) uncertainties from the determination of the lattice spacing $a$ (from the physical value of the parameter $r_{1}$ ) that are correlated between the points. The experimental average is plotted as the black point at the origin, offset slightly from the $y$-axis for clarity.
resenting its uncertainty, is approximately $2 \delta[16]^{1}$. Thus lattice spacing uncertainties are typically much more important in the determination of hyperfine splittings than

[^301]statistical errors.
We fit the hyperfine splitting as a function of lattice spacing and sea quark masses to the form:
\[

$$
\begin{align*}
f\left(a, \delta x_{l}, \delta x_{s}\right)= & f_{0} \times  \tag{3}\\
& \sum_{i j k l} c_{i j k l}\left(a m_{c}\right)^{2 i}\left(\frac{\delta x_{1}}{10}\right)^{j}\left(\frac{\delta x_{2}}{10}\right)^{k}\left(\frac{\delta x_{3}}{10}\right)^{l} \\
+ & \left(d_{0}+d_{1}\left(a m_{c}\right)^{2}\right)\left(M_{\eta_{c}, \text { latt }}-M_{\eta_{c}, \text { expt }}\right) .
\end{align*}
$$
\]

Here $f_{0}$ is the physical result, the sum over $i j k l$ allows for discretisation errors and sea quark effects and the final term allows for mistuning of the $c$ quark mass. We allow the discretisation errors, which are evident in our results, to have a scale set by the $c$ quark mass. These appear only as even powers of $a$ for staggered quarks. $\delta x_{l}$ and $\delta x_{s}$ are the mistuning of the sea quark masses:

$$
\begin{equation*}
\delta x_{q}=\frac{m_{q, \text { sea }}-m_{q, \text { phys }}}{m_{s, \text { phys }}} . \tag{4}
\end{equation*}
$$

$\delta x_{l}$ and $\delta x_{s}$ values are given for each ensemble in Table I and are taken from Appendix A of [2]. Eq. (3) includes a term for each sea quark ( $u / d$ appearing twice, and $s$ ), with the coefficients constrained to be the same so that the fit function is symmetric with respect to interchange of any two. The division by 10 is because the scale for dependence on light quark masses from chiral perturbation theory is $4 \pi f_{\pi} \approx 10 m_{s}$. We see no significant sea quark mass dependence in the hyperfine splitting. A fairly strong dependence was seen in the twisted mass calculations 10. However, at least some of that dependence could be attributed to the sea quark mass dependence of the lattice spacing, since that is determined only in the chiral limit. Here we determine the lattice spacing for each ensemble and hence separate lattice spacing dependence from physical sea quark mass effects. The sum over $i j k l$ in eq. (3) allows for the possibility of lattice spacing dependent sea quark mass effects.

We take a Bayesian prior [15] on $f_{0}$ of $0.1(1)$ and then fix $c_{0000}$ to 1 . The other $c_{i j k l}$ are given priors of $0.0 \pm 1.0$ except for the $c_{0 j k l}$ which determine the $a$-independent sea quark mass dependence. These are taken to have priors $0.0 \pm 0.33$ because we expect sea quark mass effects to be typically a factor of 3 smaller than valence quark mass effects which would have chiral perturbation theory coefficients of $\mathcal{O}(1)$. We include 5 terms in the $a$-dependence and 3 in the $\delta x$ dependence. Including additional terms makes no difference to the value for $f_{0}$ or its error. The priors for $d_{0}$ and $d_{1}$ are taken as $0.00(5)$, informed by the expectation that the hyperfine splitting should be inversely proportional to the mass, and by the effect of our mistuned $c$ mass on set 2 which agrees roughly with that expectation.

The fit gives $f_{0}=116.5(2.1) \mathrm{MeV}$, as the result for the hyperfine splitting in the absence of electromagnetism, $c$ -in-the-sea and $\bar{c} c$ annihilation. The first two affect the $\eta_{c}$ and $J / \psi$ equally and so have no effect on the hyperfine splitting. The third affects the $\eta_{c}$ more than the $J / \psi$, which has negligible width. A perturbative estimate of the shift of the $\eta_{c}$ mass resulting from its annihilation to two gluons 11 related this to the total $\eta_{c}$ width and obtained a shift downwards of the $\eta_{c}$ mass of $2.4 \mathrm{MeV}^{2}$. Using this, we have since applied a shift of $2.4(1.2) \mathrm{MeV}$ for this effect to determine the $\eta_{c}$ mass to which to tune our $c$ quark mass, as in section [II] For this purpose the impact of the shift is completely negligible, amounting to less than $0.1 \%$ of the $\eta_{c}$ mass. For the hyperfine splitting, however, this shift could be a relatively large effect. Nonperturbative calculations of the contribution of 'disconnected diagrams' to the $\eta_{c}$ mass have agreed on a small value of a few MeV for the shift from $\eta_{c}$ annihilation but obtained the opposite sign [17]. The argument is that the perturbative result may be modified significantly by the $g g$ intermediate state forming a resonance such as a glueball which is lighter in mass than the $\eta_{c}$, or a lighter hadron state. To allow for this possibility and be consistent with the nonperturbative calculations we do not apply a shift to the hyperfine splitting obtained from our fit above, but instead take an additional systematic error of 2.4 MeV , corresponding to our original shift, to allow for the effect.

Our final result for the hyperfine splitting is then:

$$
\begin{equation*}
\Delta M_{\mathrm{hyp}}=116.5(2.1)(2.4) \mathrm{MeV} \tag{5}
\end{equation*}
$$

where the errors are in turn from statistics/fitting and $\eta_{c}$ annihilation. The uncertainty from $\eta_{c}$ annihilation dominates the error. A complete error budget is given in Table III.

This is to be compared to the difference of the experimental averages of the two masses of $115.9(1.1)$

[^302]|  | $M_{J / \psi}-M_{\eta_{c}}$ | $f_{J / \psi}$ | $V_{J / \psi \rightarrow \eta_{c} \gamma}(0)$ |
| :--- | :---: | :---: | :---: |
| $\left(a m_{c}\right)^{2}$ extrapolation | 0.45 | 0.45 | 3.5 |
| statistics | 0.50 | 0.41 | 0.74 |
| lattice spacing | 1.6 | 0.42 | 0.0 |
| sea quark extrapolation | 0.29 | 0.26 | 1.3 |
| $M_{\eta_{c}}$ tuning | 0.11 | 0.09 | 0.0 |
| Z | - | 1.23 | 0.14 |
| $M_{\eta_{c}}$ annihilation | 2.1 | 0.0 | 0.0 |
| electromagnetism | 0.0 | 0.5 | 0.5 |
| Total (\%) | 2.7 | 1.5 | 3.8 |

TABLE III: Complete error budget for hyperfine splitting, leptonic width and vector form factor as a percentage of the final answer.

MeV [7. Quite a spread of results make up the average. Recent values tend to be at the lower end of the hyperfine splitting range. For example, the 2011 Belle result for the $\eta_{c}$ mass gives a hyperfine splitting of $111.5\binom{+1.6}{-2.5} \mathrm{MeV}$ [18], and a recent result from BESIII gives $112.6(0.9) \mathrm{MeV}$ [19].

## B. $\Gamma\left(J / \psi \rightarrow e^{+} e^{-}\right)$and $R_{e^{+} e^{-}}$

The amplitude, $a_{0}$, from the fit in equation (1) to our $J / \psi$ correlators is directly related to the matrix element for the local vector operator to create or destroy the ground-state vector meson from the vacuum. The vector meson decay constant, $f_{v}$, for meson $v$ is defined by:

$$
\begin{equation*}
\langle 0| \bar{\psi} \gamma^{i} \psi|v\rangle=f_{v} m_{v} \epsilon^{i} \tag{6}
\end{equation*}
$$

where $\epsilon^{i}$ is the meson polarization. $f_{v}$ for the $J / \psi$ is then determined from our lattice QCD correlators, in terms of the ground-state parameters from our fit (eq. (11) by:

$$
\begin{equation*}
\frac{f_{v}}{Z}=a_{0} \sqrt{\frac{2}{M_{0}}} \tag{7}
\end{equation*}
$$

where $Z$ is the renormalisation constant required to match the local vector current in lattice QCD used here to that of continuum QCD at each value of the lattice spacing.
$f_{v}$ is clearly a measure of the internal structure of a meson and in turn is related to the experimentally measurable leptonic branching fraction:

$$
\begin{equation*}
\Gamma\left(v_{h} \rightarrow e^{+} e^{-}\right)=\frac{4 \pi}{3} \alpha_{Q E D}^{2} e_{h}^{2} \frac{f_{v}^{2}}{m_{v}} \tag{8}
\end{equation*}
$$

where $e_{h}$ is the electric charge of the heavy quark in units of $e(2 / 3$ for $c)$. The experimental average, $\Gamma(J / \psi \rightarrow$ $\left.e^{+} e^{-}\right)=5.55(14) \mathrm{keV}$ [7] gives $f_{J / \psi}=407(5) \mathrm{MeV}$, remembering that the electromagnetic coupling constant runs with scale and using $1 / \alpha_{Q E D}\left(m_{c}\right)=134$ [20]. This can then provide a test of QCD at the $1 \%$ level. Electromagnetic corrections are small since the $J / \psi$ must decay to an odd number of photons [21].

Our results for $f_{J / \psi} / Z$ are given in Table II. The final column of that table gives the values of $Z$ determined from current-current correlators as described in Appendix B. This method uses continuum perturbation theory through $\mathcal{O}\left(\alpha_{s}^{3}\right)$ to normalise the lattice QCD correlators at small times. $Z$ then results from a combination of non-perturbative lattice QCD calculations with continuum perturbation theory in a similar approach to that of the RI-MOM scheme ${ }^{3}$ used to renormalise the currents for the same calculation using twisted mass quarks in [10]. The current-current correlator method has the advantage that we can use the same correlators from which we also extract, at large times, the nonperturbative information on the ground-state mass and decay constant. Indeed this allows some cancellation of discretisation errors apparent in the unrenormalized decay constant.

Multiplying $f_{J / \psi} / Z$ by $Z$ and then by $a^{-1}$ in GeV gives the physical results for the decay constant plotted in Figure 3. We fit these to the same function of lattice spacing and sea quark mass used for the hyperfine splitting, eq. (3). The only differences are that the prior on $f_{0}$ is taken as $0.5(5)$ in this case and the priors on the slope of the variation of $f_{J / \psi}$ with $M_{\eta_{c}}$ are taken as: $d_{0}, 0.065(5)$ and $d_{1}, 0.00(25)$. These are informed by the variation we see for the deliberately mistuned $c$ mass on set 2 and also by our extensive study of the behaviour of $f_{\eta_{c}}$ with $M_{\eta_{c}}$ in [2]. There we find a strong $a$-dependence in the slope of the decay constant with mass and so we allow for that here.

The physical result that we obtain in the continuum limit is:

$$
\begin{equation*}
f_{J / \psi}=405(6)(2) \mathrm{MeV} \tag{9}
\end{equation*}
$$

The first error is from the fit and is dominated by the error from the $Z$ factor. The second error is an estimate of systematic effects from missing electromagnetism in our lattice QCD calculation [2]. The effect of missing $c$-in-the-sea is negligible in this case. A complete error budget is given in Table III.

The leptonic width is determined by the amplitude of the ground-state that dominates the correlator at large times. We can also determine the charm contribution to $R_{e^{+} e^{-}}$through the time moments of the $J / \psi$ correlator which depend on the behaviour at short times. The moments are defined by:

$$
\begin{equation*}
G_{n}^{V}=Z^{2} C_{n}^{V}=Z^{2} \sum_{\tilde{t}} \tilde{t}^{n} \bar{C}_{J / \psi}(\tilde{t}) \tag{10}
\end{equation*}
$$

where $\tilde{t}$ is lattice time symmetrised around the centre of the lattice (see Appendix $B$ ). Results for $\left(G_{n}^{V} / Z^{2}\right)^{1 /(n-2)}$ in lattice units on each of our ensembles are given in Table IV for $n=4,6,8$ and 10 . The power $1 /(n-2)$ is

[^303]

FIG. 3: Results for the charmonium vector decay constant plotted as a function of lattice spacing. For the $x$-axis we use ( $\left.m_{c} a\right)^{2}$ to allow the $a$-dependence of our fit function (eq. (3)) (blue dashed line with grey error band) to be displayed simply. The data points have been corrected for $c$ quark mass mistuning and sea quark mass effects, but the corrections are smaller than the error bars. We do not include on the plot the deliberately mistuned $c$ mass but it is included in the fit to constrain the $c$ mass dependence. The errors shown include (and are dominated by) uncertainties from the determination of the current renormalization factor, $Z$, that are correlated between the points. The experimental average is plotted as the black point at the origin, offset slightly from the $y$-axis for clarity.
taken to reduce all the moments to the same dimension. We take the $Z$ factor for the vector current to be the same one used for the leptonic width above, determined in Appendix B. Figure 4 then shows the physical results for the moments as a function of lattice spacing. The gray bands show our fits which use the same function of lattice spacing and sea quark masses as given in eq. (3). We reduce the prior width on the lattice spacing dependent terms by a factor of 4 because the moments are not as sensitive to short distances as the leptonic width or hyperfine splitting.

The physical results that we obtain for each moment in the continuum limit are given by:

$$
\begin{align*}
\left(G_{4}^{V}\right)^{1 / 2} & =0.3152(41)(9) \mathrm{GeV}^{-1} \\
\left(G_{6}^{V}\right)^{1 / 4} & =0.6695(57)(13) \mathrm{GeV}^{-1} \\
\left(G_{8}^{V}\right)^{1 / 6} & =0.9967(65)(10) \mathrm{GeV}^{-1} \\
\left(G_{10}^{V}\right)^{1 / 8} & =1.3050(65)(6) \mathrm{GeV}^{-1} \tag{11}
\end{align*}
$$

The first error comes from the fit and the second allows for electromagnetism (e.g. photons in the final state) missing from our calculation but present in experiment. The error is estimated by substituting $\alpha_{Q E D}$ for $\alpha_{s}$ in the perturbative QCD analysis of the moments [22]. A complete error budget for our results is given in Table V.

The results agree well with the values extracted for the $q^{2}$ derivative moments, $\mathcal{M}_{k}(n=2 k+2)$, of the charm quark vacuum polarization using experimental values for

| Set | $m_{c} a$ | $\left(\frac{G_{4}^{V}}{Z^{2} a^{2}}\right)^{1 / 2}$ | $\left(\frac{G_{6}^{V}}{Z^{2} a^{4}}\right)^{1 / 4}$ | $\left(\frac{G_{8}^{V}}{Z^{2} a^{6}}\right)^{1 / 6}$ | $\left(\frac{G_{10}^{V}}{Z^{2} a^{8}}\right)^{1 / 8}$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 0.622 | $0.5399(1)$ | $1.2162(1)$ | $1.732(1)$ | $2.2780(1)$ |
| 2 | 0.63 | $0.5339(1)$ | $1.2054(1)$ | $1.7581(1)$ | $2.2584(1)$ |
| 2 | 0.66 | $0.5135(1)$ | $1.1692(1)$ | $1.7081(1)$ | $2.1941(1)$ |
| 3 | 0.617 | $0.5434(1)$ | $1.2223(1)$ | $1.7817(1)$ | $2.2888(1)$ |
| 4 | 0.413 | $0.7586(1)$ | $1.6351(1)$ | $2.3887(2)$ | $3.0952(2)$ |
| 5 | 0.273 | $1.0681(1)$ | $2.2705(2)$ | $3.3454(3)$ | $4.3601(4)$ |
| 6 | 0.193 | $1.4323(3)$ | $3.0397(5)$ | $4.4990(7)$ | $5.8738(8)$ |

TABLE IV: Results in lattice units for time moments of the $J / \psi$ correlator as defined in eq. (10). We give results for $n=4$, 6, 8 and 10 .

|  | $\left(G_{4}^{V}\right)^{1 / 2}$ | $\left(G_{6}^{V}\right)^{1 / 4}$ | $\left(G_{8}^{V}\right)^{1 / 6}$ | $\left(G_{10}^{V}\right)^{1 / 8}$ |
| :--- | :---: | :---: | :---: | :---: |
| $\left(a m_{c}\right)^{2}$ extrapolation | 0.18 | 0.18 | 0.16 | 0.16 |
| statistics | 0.05 | 0.04 | 0.03 | 0.03 |
| lattice spacing | 0.32 | 0.51 | 0.43 | 0.30 |
| sea quark extrapolation | 0.14 | 0.13 | 0.12 | 0.12 |
| $M_{\eta_{c}}$ tuning | 0.15 | 0.18 | 0.17 | 0.16 |
| Z | 1.23 | 0.61 | 0.41 | 0.31 |
| electromagnetism | 0.3 | 0.2 | 0.1 | 0.05 |
| Total (\%) | 1.3 | 0.9 | 0.7 | 0.5 |

TABLE V: Complete error budget for the time moments of the $J / \psi$ correlator as a percentage of the final answer.
$R_{e^{+} e^{-}}=\sigma\left(e^{+} e^{-} \rightarrow\right.$ hadrons $) / \sigma_{p t}$ [22, 23]. The values, extracted from experiment by [22] and appropriately normalised for the comparison to ours, are:

$$
\begin{align*}
\left(M_{1}^{\exp } 4!/\left(12 \pi^{2} e_{c}^{2}\right)\right)^{1 / 2} & =0.3142(22) \mathrm{GeV}^{-1} \\
\left(M_{2}^{\exp } 6!/\left(12 \pi^{2} e_{c}^{2}\right)\right)^{1 / 4} & =0.6727(30) \mathrm{GeV}^{-1} \\
\left(M_{3}^{\exp } 8!/\left(12 \pi^{2} e_{c}^{2}\right)\right)^{1 / 6} & =1.0008(34) \mathrm{GeV}^{-1} \\
\left(M_{4}^{\exp } 10!/\left(12 \pi^{2} e_{c}^{2}\right)\right)^{1 / 8} & =1.3088(35) \mathrm{GeV}^{-1} \tag{12}
\end{align*}
$$

Our results from lattice QCD have approximately double the error of the experimental values but together these results provide a further test of QCD to better than $1.5 \%$.

$$
\text { C. } \quad \Gamma\left(J / \psi \rightarrow \gamma \eta_{c}\right)
$$

The radiative decay of the $J / \psi$ meson to the $\eta_{c}$ requires the emission of a photon from either the charm quark or antiquark and a spin-flip, so it is an M1 transition. Because it is sensitive to relativistic corrections this rate is hard to predict in nonrelativistic effective theories and potential models (see, for example, [24, 25]) Here we use a fully relativistic method in lattice QCD with a nonperturbatively determined current renormalisation and so none of these issues apply. In addition, of course, the lattice QCD result is free from model-dependence.

The quantity that parameterises the nonperturbative QCD information (akin to the decay constant of the previous section) is the vector form factor, $V\left(q^{2}\right)$, where $q^{2}$ is the square of the 4 -momentum transfer from $J / \psi$ to


FIG. 4: Results for the 4th, 6th, 8th and 10th time moments of the charmonium vector correlator shown as blue points and plotted as a function of lattice spacing. The errors shown (the same size or smaller than the points) include (and are dominated by) uncertainties from the determination of the current renormalization factor, $Z$, that are correlated between the points. The data points have been corrected for $c$ quark mass mistuning and sea quark mass effects, but the corrections are smaller than the error bars (the value for the deliberately mistuned $c$ mass on set 2 is not shown). The blue dashed line with grey error band displays our continuum/chiral fit. Experimental results determined from $R_{e^{+} e^{-}}$(eq. (12)) are plotted as the black points at the origin offset slightly from the $y$-axis for clarity.
$\eta_{c}$. The form factor is related to the matrix element of the vector current between the two mesons by:

$$
\begin{equation*}
\left\langle\eta_{c}\left(p^{\prime}\right)\right| \bar{c} \gamma^{\mu} c|J / \psi(p)\rangle=\frac{2 V\left(q^{2}\right)}{\left(M_{J / \psi}+M_{\eta_{c}}\right)} \varepsilon^{\mu \alpha \beta \gamma} p_{\alpha}^{\prime} p_{\beta} \epsilon_{J / \psi, \gamma} \tag{13}
\end{equation*}
$$

Note that the right-hand-side vanishes unless all the vectors are in different directions. Here we use a normalisation for $V\left(q^{2}\right)$ appropriate to a lattice QCD calculation in which the vector current is inserted in one $c$ quark line only and the quark electric charge $(2 e / 3)$ is taken as a separate factor. The decay rate is then given by [8]:

$$
\begin{equation*}
\Gamma\left(J / \psi \rightarrow \eta_{c} \gamma\right)=\alpha_{Q E D} \frac{64|\vec{q}|^{3}}{27\left(M_{\eta_{c}}+M_{J / \psi}\right)^{2}}|V(0)|^{2} \tag{14}
\end{equation*}
$$

where it is the form factor at $q^{2}=0$ that contributes because the real photon is massless. $|\vec{q}|$ is the corresponding momentum of the $\eta_{c}$ in the $J / \psi$ rest-frame.


FIG. 5: A schematic diagram of the connected '3-point' function in lattice QCD for $J / \psi$ to $\eta_{c}$ radiative decay. The lines all represent $c$ quark propagators in this case. The propagator labelled 1 is the spectator quark; 2 and 3 are the initial and final active quarks respectively. 0 and $T$ label the position in time of the $\eta_{c}$ and $J / \psi$ operators. The vector current is inserted at time $t$ which takes all values between 0 and $T$.

The most recent experimental result from CLEO-c [26] of $1.98(31) \%$ for the branching fraction, combined with the total width of the $J / \psi$ of $92.9(2.8) \mathrm{keV}[7]$ gives

$$
\begin{equation*}
V(0)_{\mathrm{expt}}=1.63(14) \tag{15}
\end{equation*}
$$

where we have used $\alpha_{Q E D}=1 / 137$ and $|\vec{q}|=\left(M_{J / \psi}-\right.$ $\left.M_{\eta_{c}}\right)\left(M_{J / \psi}+M_{\eta_{c}}\right) /\left(2 M_{J / \psi}\right)$. The value of $|\vec{q}|$ from experiment is $0.1137(11) \mathrm{GeV}$ where the error comes from the uncertainty in the $\eta_{c}$ mass. $V(0)$ is then the quantity that can be calculated in lattice QCD and compared to experiment.

The radiative decay of the $J / \psi$ to $\eta_{c}$ meson needs the calculation of a ' 3 -point' function in lattice QCD. The 3 points (in lattice time) correspond to: the position of the $\eta_{c}$ operator, which we take as the origin; the position of the $J / \psi$ operator which we denote $T$ and the position of the insertion of a vector operator, $\mathcal{V}=\bar{c} \gamma_{\mu} c$, which couples to the photon at time $t . t$ varies from 0 to $T$. Sums over spatial points are implied at each time. The 'connected' correlator that we calculate is illustrated in Figure 5. Disconnected correlators are expected to be negligible here based on perturbative and phenomenological arguments 8 and we do not include them.

The 3-point function is calculated in lattice QCD by combining 3 quark propagators together with appropriate spin projection matrices. As discussed in section II for staggered quarks these $\gamma$ matrices become $\pm 1$ phases. Tastes must be combined in a staggered quark correlator so that the overall correlation function is 'tasteless'. What this means for a 3-point function is that only certain taste combinations of $J / \psi, \eta_{c}$ and $\mathcal{V}$ operators are allowed. To optimise statistical errors we need to keep to a minimum the amount of point-splitting in the operators. It is also convenient, for renormalisation purposes, to have a vector current, $\mathcal{V}$, which corresponds to a local operator (and this is also what we used for the decay constant in section III B.

We therefore choose the $\eta_{c}$ operator to be the local $\gamma_{5}$ operator (so that the $\eta_{c}$ is the Goldstone pseudoscalar with spin-taste $\gamma_{5} \otimes \gamma_{5}$ ) and the $J / \psi$ operator to be a one-link separated $\gamma_{0} \gamma_{i}$ operator in which the polarisation of the $J / \psi$ and the one-link separation are both in an orthogonal spatial direction to the polarisation of the vector current, $\mathcal{V}=\bar{c} \gamma_{k} c$ (this $J / \psi$ has spin-taste structure $\gamma_{0} \gamma_{i} \otimes \gamma_{0} \gamma_{i} \gamma_{j}$ ).

To implement this configuration is simple. The spectator quark propagator (number 1 in Figure 5 ) is generated from the default random wall at time 0 . Active propagator 2 is then generated from a source which is made from a symmetric point-splitting of propagator 1 at time $T$ patterned by a phase. For a $J / \psi$ with polarisation $x$ we take a point-splitting in the $y$ direction and phase $(-1)^{x+z}$. Active propagator 3 is made from the same default random wall as 1 . Finally 2 and 3 are combined together at $t$ by summing over space with a patterning of $(-1)^{z}$ to implement a local vector current in the $z$ direction.

To achieve the configuration corresponding to $q^{2}=0$ we keep the $J / \psi$ at rest in the frame of the lattice and give the $\eta_{c}$ an appropriate spatial momentum. The $\eta_{c}$ momentum is implemented by calculating propagator 3 with a 'twisted boundary condition' [27, 28]. If propagator 3 is calculated with boundary condition:

$$
\begin{equation*}
\chi\left(x+\hat{e}_{j} L\right)=e^{2 \pi i \theta_{j}} \chi(x) \tag{16}
\end{equation*}
$$

then the momentum of the $\eta_{c}$ meson made by combining propagators 1 and 3 with our random wall sources and summing over spatial sites at the sink is:

$$
\begin{equation*}
p_{j}=\frac{2 \pi}{L_{s}} \theta_{j} \tag{17}
\end{equation*}
$$

The boundary condition in eq. 16) is actually implemented by multiplying the gluon links in the $j$ direction by phase $\exp \left(2 \pi i \theta_{j} / L_{s}\right)$. We take $j$ to be the $y$ direction here so that the momentum is in an orthogonal direction to the polarisation of both the $J / \psi$ and $\mathcal{V}$.

The 3-point function is then given by:

$$
\begin{align*}
& C_{3 p t}(0, t, T)=\sum_{s_{T}, s_{t}} \frac{1}{4}(-1)^{x_{T}+z_{T}}(-1)^{z_{t}} \times  \tag{18}\\
& \operatorname{Tr}\left\{g(t, T)\left[g\left(T+1_{y}, 0\right)+g\left(T-1_{y}, 0\right)\right] g_{\theta}^{\dagger}(t, 0)\right\}
\end{align*}
$$

where $g$ represent staggered $c$ quark propagators, with $g_{\theta}$ computed with a phase on the gluon field, the trace is over color and sums are done over spatial sites $s_{t}$ and $s_{T}$ at $t$ and $T$. The $1 / 4$ is the taste factor for the normalisation of a staggered quark loop. The corresponding 2-point function for the $\eta_{c}$ meson is

$$
\begin{equation*}
C_{\eta_{c}, 2 p t}(0, t)=\sum_{s_{t}} \frac{1}{4} \times \operatorname{Tr}\left[g(t, 0) g_{\theta}^{\dagger}(t, 0)\right] \tag{19}
\end{equation*}
$$

| Set | $N_{\text {cfg }} \times N_{t}$ | $T$ values | $m_{c} a$ | $\begin{gathered} a M_{J / \psi} \\ \gamma_{0} \gamma_{i} \otimes \gamma_{0} \gamma_{i} \gamma_{j} \end{gathered}$ | $\begin{gathered} \hline \hline a M_{\eta_{c}} \\ \gamma_{5} \otimes \gamma_{5} \\ \hline \end{gathered}$ | $2 \pi \theta$ | $a E_{\eta_{c}}^{\theta}$ | $V_{00}^{n n}$ | $V(0) / Z$ | $Z_{f f}$ | $a^{2} q^{2}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | $2088 \times 4$ | 15,18,21 | 0.622 | 1.86084(10) | 1.79116(4) | 1.6410 | 1.79243(4) | 0.0362(2) | 1.900(11) | 0.9896(11) | $1(4) \times 10^{-5}$ |
| 2 | $2259 \times 4$ | 15,18,21 | 0.63 | 1.87972(12) | $1.80842(7)$ | 1.4007 | 1.81023(5) | 0.0368(2) | 1.897(12) | 0.9894(8) | $-7(1) \times 10^{-5}$ |
|  |  | 15,18,21 | 0.63 | 1.87962(14) | 1.80839(8) | 1.3880 | 1.81019(4) | 0.0362(4) | 1.883(20) | 0.9894(8) | $1(5) \times 10^{-5}$ |
| 4 | $1911 \times 4$ | 20,23,26,29 | 0.413 | $1.32905(9)$ | $1.28046(3)$ | 1.3327 | 1.28133(3) | 0.0348(2) | 1.876(8) | 1.0049(10) | $6(4) \times 10^{-5}$ |
|  | $\gamma_{i} \otimes \gamma_{i} \gamma_{j} \quad \gamma_{0} \gamma_{5} \otimes \gamma_{0} \gamma_{5}$ |  |  |  |  |  |  |  |  |  |  |
| 1 | $2088 \times 4$ | 15,18,21 | 0.622 | 1.86035(15) | 1.79621(4) | 1.5120 | 1.79725(4) | 0.0338(6) | 1.925(35) | 0.9896(11) | $3(5) \times 10^{-5}$ |
| 2 | $2259 \times 4$ | 15,18,21 | 0.63 | 1.87887(13) | 1.81369(6) | 1.2814 | 1.81480(5) | 0.0334(8) | 1.896(45) | 0.9894(8) | $0(4) \times 10^{-5}$ |
|  |  | 15,18,21 | 0.66 | 1.93604(15) | 1.87254(6) | 1.2490 | $1.87355(6)$ | 0.0322(8) | 1.934(42) | 0.9863(17) | $1(5) \times 10^{-5}$ |
| 4 | $1911 \times 4$ | 19,20,23,26 | 0.413 | 1.32904(11) | $1.28160(4)$ | 1.3116 | $1.28243(4)$ | 0.0342(4) | 1.872(21) | 1.0049(10) | $-2(1) \times 10^{-5}$ |

TABLE VI: Results from simultaneous fits for 3-point and 2-point correlators for $J / \psi \rightarrow \gamma \eta_{c}$ decay. The upper table gives results from our preferred jpsigamma0 method; the lower table from etacgamma0. See the text for a definition of the two methods. Column 2 gives the number of configurations and time sources for 0 on each configuration. Column 3 gives the different values of the end-point of the 3 -point function, $T$, included in the fit. The lattice $c$ quark mass and $\epsilon$ parameter are the same as those used in section III A (the lower table includes the deliberately mistuned mass on set 2 for comparison). $a M_{J / \psi}$ and $a M_{\eta_{c}}$ are the zero-momentum meson masses for the tastes of $J / \psi$ and $\eta_{c}$ mesons used here. $2 \pi \theta$ indicates the value of the phase at the boundary used to achieve the kinematics of $q^{2}=0$ in the $J / \psi \rightarrow \eta_{c}$ decay. The $a^{2} q^{2}$ values actually obtained with those kinematics are given in the final column (rows 2 and 3 of the upper table compare two different values of $a^{2} q^{2}$ close to zero). $a E_{\eta_{c}}$ gives the energy of the $\eta_{c}$ at the value of the spatial momentum corresponding to $\theta$. $V_{n n}^{00}$ from the 3 -point fit of eq 25 is given in column 9 and this is converted to a value of $V(0) / Z$ in column 10 using eq. 27). Column 11 gives the values of the renormalisation parameter, $Z$, obtained from the vector form factor method of Appendix B 2

The 2-point function for the $J / \psi$ is given by

$$
\begin{align*}
& C_{J / \psi, 2 p t}(0, t)=\sum_{s_{t}} \frac{1}{4}(-1)^{y_{0}+t_{0}}(-1)^{y_{t}+t_{t}} \times  \tag{20}\\
& \operatorname{Tr}\left[g(t, 0)\left(g^{\dagger}\left(t+1_{y}, 1_{y}\right)+g^{\dagger}\left(t-1_{y}, 1_{y}\right)+\{1 \leftrightarrow-1\}\right)\right]
\end{align*}
$$

As an alternative configuration we can take the $\eta_{c}$ operator to be the local $\gamma_{0} \gamma_{5}$ operator (so that the $\eta_{c}$ is the local non-Goldstone meson with spin-taste structure $\left.\gamma_{0} \gamma_{5} \otimes \gamma_{0} \gamma_{5}\right)$ and the $J / \psi$ operator to be a one-link separated $\gamma_{i}$ operator in which the polarisation of the $J / \psi$ and the one-link separation are both in an orthogonal spatial direction to the polarisation of the vector current, $\mathcal{V}$ (this has spin-taste structure $\gamma_{i} \otimes \gamma_{i} \gamma_{j}$ ). The 3-point function is then given by:

$$
\begin{align*}
& C_{3 p t}(0, t, T)=\sum_{s_{T}, s_{t}} \frac{1}{4}(-1)^{x_{0}+y_{0}+z_{0}}(-1)^{y_{T}}(-1)^{z_{t}} \times \\
& \operatorname{Tr}\left[g(t, T)\left(g\left(T+1_{y}, 0\right)+g\left(T-1_{y}, 0\right)\right) g_{\theta}^{\dagger}(t, 0)\right] \quad(21 \tag{21}
\end{align*}
$$

and the corresponding 2-point functions are:

$$
\begin{align*}
C_{\eta_{c}, 2 p t}(0, t)= & \sum_{s_{t}} \frac{1}{4}(-1)^{x_{0}+y_{0}+z_{0}}(-1)^{x_{t}+y_{t}+z_{t}} \times \\
& \operatorname{Tr}\left[g(t, 0) g_{\theta}^{\dagger}(t, 0)\right] . \tag{22}
\end{align*}
$$

and

$$
\begin{aligned}
& C_{J / \psi, 2 p t}(0, t)=\sum_{s_{t}} \frac{1}{4}(-1)^{x_{0}+z_{0}+t_{0}}(-1)^{x_{t}+z_{t}+t_{t}} \times \quad(23) \\
& \operatorname{Tr}\left[g(t, 0)\left(g^{\dagger}\left(t+1_{y}, 1_{y}\right)+g^{\dagger}\left(t-1_{y}, 1_{y}\right)+\{1 \leftrightarrow-1\}\right)\right] .
\end{aligned}
$$

We call this configuration the 'etacgamma0' configuration and the original configuration of eq. (19) the 'jpsigamma0' configuration. In fact, as we shall see, the jpsigamma0 configuration is to be preferred on the basis of statistical errors but the results agree between the two.

The 3-point function in both cases is calculated along with the 2 -point functions for the $\eta_{c}$ and $J / \psi$ mesons that appear in it. We use multiple time-sources for point 0 on each configuration and also multiple values for $T$. Figure 6 shows results for the 3 -point function on fine set 4 , normalising it to the product of the relevant 2 point functions. The two plots compare results for the jpsigamma0 method and the etacgamma0 method. The two differ in the amount of oscillation that is seen at the two ends of the plot. Not surprisingly the jpsigamma0 method shows more oscillation on the $J / \psi$ end ( $t$ near $T)$ since the $\eta_{c}$ in this case would not oscillate at rest. The etacgamma0 method has relatively large oscillations for the $\eta_{c}$ side but smaller oscillations on the $J / \psi$ side. In both cases statistical errors are very small enabling us to fit both normal and oscillating terms. The figure also shows how having multiple $T$ values improves our determination of the ground-state transition amplitude.

We fit the 3 -point function and 2-point functions simultaneously to a multi-exponential that determines the ground-state amplitudes accurately because it includes excited state contributions. The fit form for the 2-point functions was already given in eq. (1). Here both the $J / \psi$ and $\eta_{c}$ correlators have oscillating contributions and, in the $\eta_{c}$ case, the exponent gives the energy of the meson at momentum $p_{j}$ (eq. 17)) rather than the mass. The


FIG. 6: A plot of the ratio $C_{3 p t}(t, T) /\left(C_{2 p t, \eta_{c}}(t) C_{2 p t, J / \psi}(T-\right.$ $t)$ ) for the three values of $T$ on the fine ensemble, set 4 and for our two different methods. Lines join the points (which have statistical errors on them) for clarity. We only include points in the central region of $t$ i.e. $t \geq 5$ or $t \leq T-5$. The pink shaded band shows the ratio of fit parameters $V_{00}^{n n} / a_{0} b_{0}$ which is the ground-state contribution to this ratio. These come from a fit that included 6 normal exponentials and 5 oscillating ones (which produce the oscillations evident in the figure). The top plot shows the results for the case where $\gamma_{0}$ is included in the $J / \psi$ operator (jpsigamma0 method) and the lower plot shows the results for the case where $\gamma_{0}$ is included in the $\eta_{c}$ operator (etacgamma0 method).
fit form for the 3-point function is then:

$$
\begin{aligned}
& C_{3 p t}(t, T)= \\
& \sum_{i_{n}, j_{n}} a_{i_{n}} \operatorname{fn}\left(E_{a, i_{n}}, t\right) V_{i_{n}, j_{n}}^{n n} b_{j_{n}} \operatorname{fn}\left(E_{b, j_{n}}, T-t\right) \\
& -\sum_{i_{n}, j_{o}} a_{i_{n}} \operatorname{fn}\left(E_{a, i_{n}}, t\right) V_{i_{n}, j_{o}}^{n o} \tilde{b}_{j_{o}} \mathrm{fo}\left(\tilde{E}_{b, j_{o}}, T-t\right) \\
& -\sum_{i_{o}, j_{n}} \tilde{a}_{i_{o}} \mathrm{fo}\left(\tilde{E}_{a, i_{o}}, t\right) V_{i_{o}, j_{n}}^{o n} b_{j_{n}} \mathrm{fn}\left(E_{b, j_{n}}, T-t\right) \\
& +\sum_{i_{o}, j_{o}} \tilde{a}_{i_{o}} \mathrm{fo}\left(\tilde{E}_{a, i_{o}}, t\right) V_{i_{o}, j_{o}}^{o o} \tilde{b}_{j_{o}} \mathrm{fo}\left(\tilde{E}_{b, j_{o}}, T-t\right)
\end{aligned}
$$

and, again:

$$
\begin{align*}
\mathrm{fn}(E, t) & =e^{-E t}+e^{-E\left(L_{t}-t\right)} \\
\mathrm{fo}(E, t) & =(-1)^{t / a} \mathrm{fn}(E, t) \tag{25}
\end{align*}
$$

with $L_{t}$ again the time extent of the lattice. Here $n$ denotes the normal contributions and $o$ the contributions from oscillating states. The ground-state energies/masses that we need are $E_{\eta_{c}, 0}$ and $E_{J / \psi, 0}=M_{J / \psi}$ and the matrix element between them that is proportional to $V_{0,0}^{n n}$. By matching to a continuum correlator with a relativistic normalisation of states and allowing for a renormalisation of the lattice vector current we see that:

$$
\begin{equation*}
\left\langle\eta_{c}\right| V|J / \psi\rangle=2 Z \sqrt{M_{J / \psi} E_{\eta_{c}}} V_{0,0}^{n n} . \tag{26}
\end{equation*}
$$

The vector form factor that we need, $V(0)$, is then, from eq. (13), given by:

$$
\begin{equation*}
\frac{V(0)}{Z}=\frac{M_{J / \psi}+M_{\eta_{c}}}{2 M_{J / \psi} p_{j}} 2 \sqrt{M_{J / \psi} E_{\eta_{c}}} V_{0,0}^{n n} \tag{27}
\end{equation*}
$$

with $p_{j}$ from eq. 17). The determination of $Z$ will be discussed below.

To perform the joint fit to the 3pt correlators using eq. (25) and the 2 pt correlators using eq.(11) we use the same approach as outlined in section III A. For both the $\eta_{c}$ and $J / \psi$, the prior for the ground-state mass comes from the effective mass of the correlator. We use priors of 600 MeV with a width of 300 MeV for the difference in mass between the ground state and the lowest oscillating mass and between all radial excitations, both normal and oscillating. The 2 -point amplitudes, $a_{i}$ and $b_{i}$, have prior widths of 0.5 and the 3 -point amplitudes, $V_{i j}$, have widths of 0.25 . We omit $t$ values below a certain $t_{\text {min }}$ to reduce the effect of excited states. $t_{\min }=4(5)$ for the coarse(fine) lattices for the etacgamm0 method and 6 for the jpsigamm0 method.

Table VI gives our results from fits that include 6 normal exponentials and 5 oscillating. We work on ensembles 1,2 and 4 of Table $\square$ but using more configurations than in section III A to reduce statistical errors. Table VI gives the number of configurations and time sources as well as the values of $T$ used in the 3 -point functions. It is important to use both even and odd values of $T$ to separate clearly the normal and oscillating contributions. Having determined the mass of the local non-Goldstone $\eta_{c}$ and 1-link vector from separate 2-point function fits we then determine the value of $\theta$ needed to achieve $q^{2}=0$. The final fits are done as a simultaneous fit to the 3-point function and 2-point functions for zero momentum and finite momentum $\eta_{c}$ and zero momentum $J / \psi$.

The key parameters to be determined from the fit, as discussed above, are the ground-state masses of the $\eta_{c}$ and $J / \psi$, the ground state energy at non-zero momentum of the $\eta_{c}$ and the ground-state to ground-state amplitude of the 3-point function. Our fit returns excited


FIG. 7: Results for the vector form factor at $q^{2}=0$ for $J / \psi \rightarrow$ $\eta_{c}$ decay plotted as a function of lattice spacing. The filled blue circles are from our preferred jpsigamma0 method; the open blue circles are from the etacgamma 0 method. For the $x$-axis we use $\left(m_{c} a\right)^{2}$ to allow the $a$-dependence of our fit function to be displayed simply (blue dashed line and grey band). The fit is to results from the jpsigamma0 method. The errors shown include statistical errors and errors from the $Z$ factor. The experimental result extracted from the branching fraction for $J / \psi \rightarrow \gamma \eta_{c}$ is plotted as the black point offset slightly from the origin for clarity.
state to ground-state and oscillating to ground state amplitudes also. Most of these do not have a significant signal. Indeed the excited state to ground state amplitudes are very small, as expected since they correspond to a hindered M1 transition. A non-zero result is seen for the transition between the oscillating partner of the $\eta_{c}$ (in the etacgamma0 method) and the $J / \psi$. This corresponds to the E1 $\chi_{c 0}$ to $J / \psi$ decay, but not at the correct kinematics for that decay. Likewise a signal is seen for E1 $h_{c} \rightarrow \eta_{c}$ decay in jpsigamma0 method. We will discuss these transitions further elsewhere.

From eq. 27) we can determine $V(0)$ given a value for $V_{00}^{n n}$ and a renormalisation factor, $Z$. For $Z$ we use the fully nonperturbative vector form factor method described in Appendix B2 which normalises the local charm-charm vector current that we are using here by demanding that its form factor is 1 between identical mesons at $q^{2}=0$. This requires a non-staggered spectator quark and we use NRQCD for this. The determination of $Z_{f f}$ then needs the calculation of the form factor of the temporal component of the vector current between two $B_{c}$-like mesons (the mesons do not have to be real $B_{c}$ mesons) at rest. $Z_{f f}$ can be determined with a statistical uncertainty of $0.1 \%$ this way. Details are given in Appendix B 2.

The values for $Z$ are given in Table IX of Appendix B 2 and the values we use here are reproduced in Table VI along with our results for $V_{00}^{n n}, V(0) / Z$ and the $\eta_{c}$ and $J / \psi$ masses and energies. The table is divided into two
with the upper results from the jpsigamma0 method and the lower results from the etacgamma0 method. The two methods give results for $V(0) / Z$ in good agreement, but the jpsigamma0 results are statistically more accurate. This is then our preferred method and the one that we will use for our final result. The agreement between the two methods to within the $2 \%$ statistical errors is a strong test of the control of discretisation errors in the HISQ formalism.

Table IXalso gives results that allow us to test to what extent $V(0)$ depends on $m_{c}$ and the precise tuning of $q^{2}$ to zero. On set 2 we have deliberately mistuned the $c$ quark mass by $5 \%$ and see that it makes no significant difference to $V(0)$ within our $2 \%$ statistical errors. $q^{2}$ is tuned to zero typically within our statistical errors of $(10 \mathrm{MeV})^{2}$. On set 2 comparison between two different values of $q^{2}$ shows no effect within our $1 \%$ statistical errors. We use the value closest to $q^{2}=0$ in our fits below. These are both good tests of the robustness of our results to the tuning of parameters.

Figure 7 shows our results for $V(0)$ plotted as a function of the lattice spacing. To determine the physical value we use a fit similar to that for the hyperfine splitting and leptonic decay constant given in eq. 3. We simplify the fit slightly in dropping the tuning for the physical $c$ mass since our results in Table VI show negligible dependence on the $c$ quark mass. We take the prior on the physical value to be $2.0(0.5)$ and allow for terms in $\left(m_{c} a\right)^{2 i}$ up to $i=5$. We take the prior on the leading $\left(m_{c} a\right)^{2}$ term to be $0.0(3)$ since tree-level $a^{2}$ errors are removed in the HISQ action. We take linear and quadratic terms in $2 \delta x_{l}+\delta x_{s}$ and allow $a^{2}$ dependence multiplying the linear term.

The physical value for $V(0)$ from the fit is $1.90(7)$ from the jpsigamma0 method. The etacgamma0 method gives a result in good agreement with a very similar error. The error is dominated by that from the extrapolation in the lattice spacing. In fact there is no visible lattice spacing dependence in our results and it could be argued that, in a transition from $J / \psi$ to $\eta_{c}$ that probes relatively low momenta, the relevant scale for discretisation errors is well below $m_{c}$. However, to be conservative, we allow discretisation errors to depend on $\left(m_{c} a\right)^{2}$ and allow for multiple powers to appear.

We have also tested extrapolations of $V(0)$ to the physical point using alternative definitions of the renormalisation of the current. We get the same answer using $Z_{f f}$ values taken from $B_{c} \rightarrow B_{c}$ form factors with a heavier $b$ quark mass, as given in Appendix B 2. We also get a result in good agreement if we use values for $Z$ from $Z_{c c}$ given in Appendix B 1 .

Our physical result for $V(0)$ is for a world that does not include electromagnetism, $c$-in-the-sea or allow for $\eta_{c}$ annihilation. The effect of missing electromagnetism is similar to that for the decay constant and so we allow the same additional systematic error of $0.5 \%$. We expect $c$-in the sea effects to be negligible, as for the decay constant. $\eta_{c}$ annihilation affects the mass difference between


FIG. 8: A comparison of results for the charmonium hyperfine splitting from lattice QCD with experiment. We show only results that include sea quarks and make use of multiple lattice spacings to derive a continuum value. The experimental average [7] is given at the top, followed by the result for HISQ quarks from this paper. The Fermilab clover [29] and twisted mass [10] results follow. Neither of these lower two results include an error for missing $\eta_{c}$ annihilation effects. This error is the dominant error for our calculation. Here we show our error bar excluding this effect as a solid line and the total error including this effect as a dotted line.
the $J / \psi$ and $\eta_{c}$ (as discussed in section III A) and therefore affects the momentum of the $\eta_{c}$ that corresponds to $q^{2}=0$ for this decay. Equivalently it means that the real $q^{2}=0$ point corresponds to a non-zero $q^{2}$ in our calculation. Since we allow an uncertainty in the $\eta_{c}$ mass of 2.4 MeV (Table III) this corresponds to an uncertainty around $q^{2}=0$ of $6 \times 10^{-6} \mathrm{GeV}^{2}$, keeping the spatial momentum fixed. From Table VI we see that this would produce a negligible change in $V(0)$, not visible beneath our statistical errors. In addition we can use information from [8] which used results at different $q^{2}$ values to extrapolate to $q^{2}=0$ albeit in the quenched approximation. The $q^{2}$ dependence gave a change in $V\left(q^{2}\right)$ from $V(0)$ of $20 \%$ when $q^{2}$ was $1 \mathrm{GeV}^{2}$. From this it is clear that effects from a slight mistuning because of $\eta_{c}$ annihilation effects should be completely negligible. We take as our final result then:

$$
\begin{equation*}
V(0)=1.90(7)(1) \tag{28}
\end{equation*}
$$

The complete error budget is given in Table III.


FIG. 9: A comparison of results for the decay constant of the $J / \psi$ from lattice QCD with experiment. We include only results that include sea quarks and make use of multiple lattice spacings to derive a continuum value. The experimental average [7] is given at the top, followed by the result for HISQ quarks from this paper. The twisted mass [10] results follow.

## IV. DISCUSSION

Figure 8 compares our result for the charmonium hyperfine splitting to experiment and to that from other lattice QCD calculations. We only show results that have been obtained including sea quark effects and making use of multiple lattice spacing values to derive a physical continuum result. Values are also given for different forms of the clover action in $30-33$ but either at only one value of the lattice spacing or without giving a value from continuum extrapolation. Some of these latter calculations obtain values well below experiment because of the large discretisation errors, particularly for the hyperfine interaction, in the clover formalism.

Our result agrees well with experiment and is more accurate than earlier values, especially since earlier values do not generally include any error for missing $\eta_{c}$ annihilation effects.

Figure 9 similarly compares our result for $f_{J / \psi}$ to that from twisted mass quarks including only $u$ and $d$ quarks in the sea [10] and to experiment (from eq. (8)). Both lattice results agree well with experiment at the $2 \%$ level of accuracy achieved. Our value for $f_{J / \psi}$ gives a value for $\Gamma\left(J / \psi \rightarrow e^{+} e^{-}\right)$of $5.48(16) \mathrm{keV}$ using eq. (8).

Figure 10 shows the same comparison for the vector form factor at $q^{2}=0, V(0)$, for $J / \psi \rightarrow \eta_{c} \gamma$ decay. Our result here using HISQ quarks and including $u, d$ and $s$ quarks in the sea agrees well, at the $4 \%$ level of accuracy achieved, with the result using twisted mass quarks and including only $u$ and $d$ sea quarks.


FIG. 10: A comparison of results for the vector form factor, $V(0)$ for $J / \psi \rightarrow \eta_{c} \gamma$ from lattice QCD with experiment. We include only results that include sea quarks and make use of multiple lattice spacings to derive a continuum value. The experimental result [26] is given at the top, followed by the result for HISQ quarks from this paper. The twisted mass 10 results follow.

The value of $V(0)$ extracted from the experimental branching fraction [26] is $1.7 \sigma$ lower than the lattice numbers where $\sigma$ is dominated by the $8 \%$ uncertainty from experiment. This situation is an improvement over that before the CLEO measurement [8]. However, it is clear that a more stringent test of QCD would be possible with a smaller experimental error for the $J / \psi \rightarrow \eta_{c} \gamma$ branching fraction and this may become possible with BES III although it is a challenging mode [34, 35].

Our value for $V(0)$ corresponds to a width for $J / \psi \rightarrow$ $\gamma \eta_{c}$ of $2.49(18)(7) \mathrm{keV}$ using eq. (14). The first error is from our result and the second from the experimental error in $|\vec{q}|$. Note that in using eq. (14) we put in the experimental masses for the $J / \psi$ and $\eta_{c}$. This is appropriate because these factors are kinematic ones and therefore should be taken to match the experiment. What we calculate in lattice QCD is $V(0)$. In fact, as discussed above, we have good agreement between our results and experiment for $M_{J / \psi}-M_{\eta_{c}}$ and so the kinematic factors would also be correct from lattice QCD. However, extra uncertainty would be introduced by using the lattice QCD results and that is not necessary or appropriate. Our result for the decay width corresponds to a branching fraction for $J / \psi \rightarrow \eta_{c}$ of $2.68(19)(11) \%$, where the first error is from our calculation and the second from experiment, including the experimental width of the $J / \psi$.

Figures 2,3 and 7, which show our results as a function of lattice spacing, confirm that discretisation errors are small (although visible) for the HISQ formalism and that
the approach to the continuum limit is well-controlled. This is discussed further in Appendix C where we compare the dependence on lattice spacing to that for twisted mass quarks 10.

## V. CONCLUSIONS

We have given results for 3 key quantities associated with the $J / \psi$ meson from lattice QCD, for the first time including the effect of all three $u, d$ and $s$ quarks in the sea. The quantities are the mass difference with its pseudoscalar partner, the $\eta_{c}$ meson, the decay constant and the vector form factor at $q^{2}=0$ for $J / \psi \rightarrow \eta_{c}$ decay.

Our first key result is for the $J / \psi$ decay constant. We obtain:

$$
\begin{equation*}
f_{J / \psi}=405(6) \mathrm{MeV} \tag{29}
\end{equation*}
$$

leading to $\Gamma\left(J / \psi \rightarrow e^{+} e^{-}\right)=5.48(16) \mathrm{keV}$. This is to be compared to the experimental result of $\Gamma\left(J / \psi \rightarrow e^{+} e^{-}\right)$ $=5.55(14) \mathrm{keV}$ [7]. We have therefore achieved a $4 \%$ test of lattice QCD from an electromagnetic decay rate (a $2 \%$ test from the decay constant), that does not suffer from CKM uncertainties. This is itself a stringent test of QCD and one for which lattice QCD is absolutely necessary; $f_{J / \psi}$ could not be calculated this accurately with any other method. At the same time we are able to verify that the time-moments of the $J / \psi$ correlator agree as they should with results for the charm contribution to $\sigma\left(e^{+} e^{-} \rightarrow\right.$ hadrons $)$ extracted from experiment. This is a test of QCD to better than $1.5 \%$.

Our $f_{J / \psi}$ result is a critically important test for our calculations that determine the decay constants of the $D_{s}$ [2, 36] and the $D$ [36, 37] to a similar level of precision. In particular it tests the HISQ formalism for $c$ quarks [11] even more stringently than in the $D$ and $D_{s}$ cases because the $J / \psi$ contains two $c$ quarks and is a smaller meson, more sensitive to discretisation effects on the lattice. Combined with our earlier work on using the HISQ formalism for light quarks in $f_{\pi}$ and $f_{K}$ [13, 36, 38], our result for $f_{J / \psi}$ provides compelling evidence that we have the systematic errors in $f_{D_{s}}$ and $f_{D}$ under control.

We can improve our result for $f_{J / \psi}$ further in future by using the vector form factor method of renormalisation rather than the current-current correlator method. This will only be useful if improved experimental results become available. This is expected from BESIII [35].

A further test of QCD/Lattice QCD comes from the $J / \psi$ mass. We find:

$$
\begin{equation*}
M_{J / \psi}-M_{\eta_{c}}=116.5 \pm 3.2 \mathrm{MeV} \tag{30}
\end{equation*}
$$

giving $M_{J / \psi}=3.0975(32)(11) \mathrm{GeV}$ where the second error comes from the experimental average for $M_{\eta_{c}}$ [7]. Experiment gives $M_{J / \psi}=3.0969 \mathrm{GeV}$. This is another strong test of lattice QCD, and indeed QCD, against experiment to be compared to that of the determination
of $M_{D_{s}}$ [2] and $M_{D}$ [3]. The hyperfine splitting is a relatively small relativistic correction in the broader context of charmonium meson masses and the fact that we can do this well (with no free parameters) is because the HISQ formalism is such a highly improved relativistic formalism. This is underlined by a study of the meson dispersion relation (and associated 'speed of light') in Appendix C. In fact our error on $M_{J / \psi}$ is dominated by uncertainties from the effect of annihilation of the $\eta_{c}$ meson to gluons, and it is important to pin these down more accurately.

Our third result for the $J / \psi$ is that for its M1 radiative decay mode to the $\eta_{c}$. We find:

$$
\begin{equation*}
\Gamma\left(J / \psi \rightarrow \gamma \eta_{c}\right)=2.49 \pm 0.19 \mathrm{keV} \tag{31}
\end{equation*}
$$

to be compared to the current experimental value of $1.84(30) \mathrm{keV}$ [26]. The agreement is reasonably good, but the experimental error is large and the lattice QCD result would allow a much stronger test of QCD if this were reduced. This should be possible at BESIII 34]. Since the error in our lattice QCD result is dominated by the continuum extrapolation it will be improved in calculations on superfine and ultrafine lattices as we have done for the decay constant, and $2 \%$ errors should also be achievable here. Again, this is only possible in lattice QCD.

The $J / \psi \rightarrow \gamma \eta_{c}$ decay rate is another test of QCD , along with our leptonic decay constant, that is free of CKM uncertainties. It provides a validation of semileptonic decay rate calculations for $D$ and $D_{s}$ mesons 39 43, that also use HISQ quarks as well as a test of our techniques for nonperturbative current renormalisation that we are using for a range of semileptonic and radiative decays 41-43].

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FIG. 11: Difference in mass in MeV for different meson 'tastes' for the $\eta_{c}$ and $J / \psi$ used here, plotted against the square of the lattice spacing. Red open circles show the mass difference between the local non-Goldstone and goldstone $\eta_{c}$ mesons. For the vector we have the mass difference between the local $J / \psi$ meson and the 1 -link $\gamma_{i} \otimes \gamma_{i} \gamma_{j}$ vector (blue crosses) and the 1 -link $\gamma_{0} \gamma_{i} \otimes \gamma_{0} \gamma_{i} \gamma_{j}$ vector (blue open triangles). The local $J / \psi$ meson is the lighter in both cases. Results are for sets 1, 2 and 4 from Tables II and VI Errors are statistical.

## Appendix A: Taste effects in staggered mesons

Each staggered meson comes in 16 different tastes, most easily seen in terms of naive quark operators made with different point splittings:

$$
\begin{equation*}
J_{n}^{(s)}=\bar{\psi}(x) \gamma_{n} \psi(x+s) \tag{A1}
\end{equation*}
$$

Here $s$ is a 4-dimensional vector with 0 or 1 in each component. The different $J_{n}^{(s)}$ operators are orthogonal to each other. To work out the corresponding staggered quark correlators we need the staggering matrix, $\Omega(x)$. In our convention this is:

$$
\begin{equation*}
\Omega(x)=\prod_{\mu=1}^{4}\left(\gamma_{\mu}\right)^{x_{\mu}} \tag{A2}
\end{equation*}
$$

with $\gamma_{4} \equiv \gamma_{0}$. Then the connection between naive quark propagators, which carry a spin index, and staggered quark propagators, which do not, is:

$$
\begin{equation*}
S_{F}(x, y) \equiv\langle\psi(x) \bar{\psi}(y)\rangle_{\psi}=g(x, y) \Omega(x) \Omega^{\dagger}(y) \tag{A3}
\end{equation*}
$$

To work out the phases that appear in the correlator of a particular taste we then simply have to calculate spin traces over products of $\Omega$ and $\gamma_{n}$ factors, see, for example, 11].

Here we use two different tastes for the $\eta_{c}$ and three for the $J / \psi$ and they all have slightly different masses. The mass differences between the different tastes of a

|  | $c_{n}^{(0)}$ | $c_{n}^{(1)}$ | $c_{n}^{(2)}$ | $c_{n}^{(3)}$ | $c_{n}^{(4)} \ldots$ |
| :--- | :--- | :--- | :--- | :--- | :--- |
| $n=4$ | 1.0 | 0.235 | 0.354 | -0.187 | $0.0(5) \ldots$ |
| $n=6$ | 1.0 | 0.246 | 0.460 | 0.198 | $0.0(5) \ldots$ |
| $n=8$ | 1.0 | 0.253 | 0.563 | 0.511 | $0.0(5) \ldots$ |

TABLE VII: The perturbative series 45-49 for the ratio $r_{n+2}^{P} / r_{n}^{V}$ for different moments, $n$, in continuum QCD perturbation theory. $c_{n}^{(i)}$ is the coefficient of $\alpha \frac{i}{M S}(\mu=m) ; c_{n}^{(0)}$ is 1.0 for all cases, by definition. $c_{n}^{(i)}$ for $i>3$ were included in the determination of $Z$, allowing for a coefficient of $0.0 \pm 0.5$.
given meson, however, vanish as $\alpha_{s}^{2} a^{2}$. For the $\eta_{c}$ we use the Goldstone meson (in spin-taste notation this is the $\gamma_{5} \otimes \gamma_{5}$ meson) and the local non-Goldstone meson (the $\gamma_{0} \gamma_{5} \otimes \gamma_{0} \gamma_{5}$ meson), which are the first two mesons on the ladder of pseudoscalar tastes. We show the mass difference between them in Figure 11 for coarse and fine lattices. The mass difference amounts on the coarse lattices to a little less than 10 MeV (for a 3 GeV particle) and clearly falls with $a^{2}$ as expected. For the $J / \psi$ we use the local vector $\left(\gamma_{i} \otimes \gamma_{i}\right)$ and two 1-link operators which have a point-splitting in an orthogonal direction to the polarisation $\left(\gamma_{i} \otimes \gamma_{i} \gamma_{j}\right.$ and $\left.\gamma_{0} \gamma_{i} \otimes \gamma_{i} \gamma_{j}\right)$. Note that these are not taste-singlet vectors. The mass difference between tastes for mesons of other $J^{P C}$ is typically much smaller than for pseudoscalars and that is clear here. Figure 11 shows that the mass difference for the vectors is $1-2 \mathrm{MeV}$ on the coarse lattices and not resolvable on the fine lattices.

In Section III C we showed results for $J / \psi \rightarrow \gamma \eta_{c}$ using different tastes of $J / \psi$ and $\eta_{c}$ at the two ends of the 3point function. No difference was seen in the vector form factor at $q^{2}=0$ in the two cases, either on the coarse or fine lattices (within our statistical errors of $2 \%$ ). This is another demonstration that taste effects are very small with HISQ quarks.

## Appendix B: Determining nonperturbative $Z$ factors for local vector currents

## 1. The current-current renormalization method

Time-moments of lattice QCD correlators for zeromomentum heavyonium mesons can be compared very accurately 50 to continuum QCD perturbation theory [45-49] developed for the analysis of the $e^{+} e^{-}$annihilation cross-section. This has been used with pseudoscalar meson correlators made with HISQ quarks to extract $c$ and $b$ masses and $\alpha_{s}$ to better than $1 \%$ [51. These results used the goldstone pseudoscalar correlator, which is absolutely normalised because of the HISQ PCAC relation. Here we apply the same techniques to vector meson correlators but use it to determine the renormalisation factor, $Z$, required for the lattice vector current to match the continuum current.

The time moments of our lattice QCD correlators are

| Set $m_{c} a$ | $Z(4)=Z_{c c} Z(6)$ | $Z(8)$ |  |  |
| :--- | :--- | :--- | :--- | :--- |
| 1 | 0.622 | $0.979(12)$ | $0.945(14)$ | $0.927(17)$ |
| 2 | 0.63 | $0.979(12)$ | $0.945(14)$ | $0.926(17)$ |
| 2 | 0.66 | $0.974(12)$ | $0.941(14)$ | $0.921(17)$ |
| 4 | 0.413 | $0.983(12)$ | $0.953(14)$ | $0.953(17)$ |
| 5 | 0.273 | $0.986(12)$ | $0.970(14)$ | $0.975(18)$ |
| 6 | 0.193 | $0.990(12)$ | $0.982(14)$ | $0.986(18)$ |

TABLE VIII: Renormalisation constants determined from the current-current correlator method on each configuration set used for the determination of $f_{J / \psi}$. The $Z$ value we use is that from moment 4. The errors include an estimate of effects from a gluon condensate contribution, and unknown fourth order and higher terms in continuum perturbation theory. The errors are highly correlated between configuration sets (to better than $1 \%$ of the error). For set 2 we include both the tuned value of $a m_{c}(0.63)$ and the heavier, detuned, value ( 0.66 ). Very little difference is seen between them.
defined as:

$$
\begin{equation*}
C_{n}^{V}=\sum_{\tilde{t}} \tilde{t}^{n} \bar{C}_{J / \psi}(\tilde{t}) \tag{B1}
\end{equation*}
$$

and

$$
\begin{equation*}
C_{n}^{P}=\sum_{\tilde{t}} \tilde{t}^{n}\left(a m_{c}\right)^{2} \bar{C}_{\eta_{c}}(\tilde{t}) \tag{B2}
\end{equation*}
$$

where $\tilde{t}$ is a symmetrised version of $t$ around the centre of the lattice, i.e. going forward in time, $\tilde{t}$ runs from 0 to $L_{t} / 2$ and then from $-L_{t} / 2+1$ to -1 . The extra factor of $\left(a m_{c}\right)^{2}$ in the pseudoscalar case is to make a correlator moment which is finite as $a \rightarrow 0$. For both correlators we expect the small $n$ moments to behave perturbatively, since they probe small times. Then our match to continuum perturbation theory is:

$$
\begin{equation*}
C_{n}^{P}=\frac{g_{n}^{P}\left(\alpha_{\overline{M S}}(\mu), \mu / m_{c}\right)}{\left(a m_{c}(\mu)\right)^{n-4}}+\mathcal{O}\left(\left(a m_{c}\right)^{m}\right) \tag{B3}
\end{equation*}
$$

where $g_{n}$ is the continuum QCD perturbation theory series in the $\overline{M S}$ scheme [45]49]. For the vector correlator a $Z$ factor is needed to multiply the lattice current and so:

$$
\begin{equation*}
C_{n}^{V}=\frac{1}{Z^{2}} \frac{g_{n}^{V}\left(\alpha_{\overline{M S}}(\mu), \mu / m_{c}\right)}{\left(a m_{c}(\mu)\right)^{n-2}}+\mathcal{O}\left(\left(a m_{c}\right)^{m}\right) \tag{B4}
\end{equation*}
$$

$Z$ is then a function of the bare lattice strong coupling constant at each lattice spacing and so this match must be performed separately on each ensemble. By taking the ratio of pseudoscalar and vector moments we can cancel the factors of the quark mass. In fact we also divide each moment by its tree-level value (calculated with the gluon fields set to 1) to reduce discretisation errors, i.e. instead of $C_{n}$ we use $R_{n}$ where

$$
\begin{equation*}
R_{n}=\frac{C_{n}}{C_{n}^{(0)}} \tag{B5}
\end{equation*}
$$

and also take the same ratio, calling it $r_{n}$, in the continuum perturbation theory. Finally $Z$ is given by:

$$
\begin{equation*}
Z(n)=\sqrt{\frac{R_{n+2}^{P} / R_{n}^{V}}{r_{n+2}^{P} / r_{n}^{V}}} \tag{B6}
\end{equation*}
$$

Table VII gives the perturbative coefficients for the series in $\alpha_{\overline{M S}}(m)$ for $r_{n+2}^{P} / r_{n}^{V}$. This is known to 4loops $\left(\alpha_{s}^{3}\right)$ and we include the possibility of unknown higher order terms (to 20th order) with prior values for the coefficients of $0 \pm 0.5$. We take $\mu=m$ but including the possibility of higher order corrections means that the results are almost completely insensitive to $\mu$. We also allow for gluon condensate contributions taking $\alpha_{s} G^{2} / \pi=0 \pm 0.012 \mathrm{GeV}^{4}$. This increases the errors on the determination of the $Z$ values as $n$ increases.

Table VIII gives the results for $Z$ on each ensemble and for moments 4,6 and 8 . The differences between the $Z$ values on a given ensemble arise from discretisation errors. We take our final result for use in section IIIB from moment 4 (and so these numbers are reproduced in Table II) since, even though discretisation errors fall as the moment number increases, the errors from the gluon condensate rise more steeply. The error in $Z(4)$ is around $1 \%$. It is dominated by the uncertainty in higher orders in perturbation theory and so strongly correlated from one lattice spacing to the next. We have checked that we obtain the same final result for $f_{\psi}$ using $\mathrm{Z}(6)$ (but with an error of $1.6 \%$ rather than $1.4 \%$ ).

## 2. The vector form factor method

Vector currents can be normalised completely nonperturbatively by requiring that the vector form factor at $q^{2}=0$ between two identical mesons be 1 since this would be true for a conserved vector current. We use this to normalise the staggered taste-singlet 1-link vector current between two mesons made of staggered quarks in 41. Here, however, we want to normalise the tastenonsinglet local staggered vector current, and we cannot do this using a 3-point function made entirely of staggered quarks. We have to include a non-staggered (and non-doubling) spectator quark in order to remove the requirement for overall taste-cancellation in the 3-point function 52. The Fermilab Lattice/MILC collaboration use this method [53] with a clover spectator quark to normalise a light staggered vector current for the nonperturbative part of their mixed perturbative/nonperturbative approach to normalising the clover-staggered operators for heavy-light meson decay constants. Here we use an NRQCD spectator quark to normalise the local charm staggered vector current. In fact we can use any NRQCDlike action for the spectator since it does not need to correspond to a physical quark. However, for simplicity we do use the NRQCD action developed for our NRQCDlight spectrum calculations [3].

To combine an NRQCD (or other non-staggered) quark with a staggered quark we convert it to a naive quark 52],


FIG. 12: The ratio of the 3 -point function for the ' $B_{c}$ ' to ' $B_{c}$ ' vector form factor to the ' $B_{c}$ ' 2 -point function against the source-current separation, $t / a$. The top plot shows results for $m_{b} a=2.0$ on fine lattices, set 4 , for various values of $T$. Lines join the points for clarity. The shaded red band gives our fit result for the ground state matrix element. The lower plot shows results, also on set 4 , for two different values of $m_{b} a$. The shaded red and blue bands show the fit results for the ground state matrix elements.
re-instating the spin degree of freedom as in eq. A3). A pseudoscalar meson correlator which, with two idential quarks, would simply be the sum over spins and colors of the squared modulus of the propagator, becomes in this case:

$$
\begin{equation*}
C_{Q q}(t)=\sum_{\vec{x}, \vec{y}} \operatorname{Tr}\left\{G(x, y) \Omega(y) g^{\dagger}(x, y) \Omega^{\dagger}(x)\right\} \tag{B7}
\end{equation*}
$$

The trace is over spin and color but separates since the staggered propagator, $g(x, y)$, has no spin and $\Omega$ no color. Then:

$$
\begin{equation*}
C_{Q q}(t)=\sum_{\vec{x}, \vec{y}} \operatorname{Tr}_{c}\left\{\operatorname{Tr}_{s}\left[\Omega^{\dagger}(x) G(x, y) \Omega(y)\right] g^{\dagger}(x, y)\right\} \tag{B8}
\end{equation*}
$$

This makes clear that we can transfer the $\Omega$ matrices to the non-staggered quark propagator, $G(x, y)$, and this allows us, as shown in [14, to combine staggered and nonstaggered quarks from random wall sources. We simply
make the source of the non-staggered quark the product of $\Omega(y)$ (where $y$ runs over a time slice at the source) with the random number at each $y$ value in the random wall, convoluted with smearing functions if required. At the sink we multiply by $\Omega^{\dagger}$ before tracing over spins to combine with the spinless staggered quark propagator. Here we develop this method further for 3-point functions.

For the matrix element of the temporal charm-charm vector current between identical charmed pseudoscalar mesons, at rest, we have:

$$
\begin{equation*}
\left\langle P_{c}\right| V_{t}\left|P_{c}\right\rangle=2 m_{P_{c}} f_{+}(0) \tag{B9}
\end{equation*}
$$

and we can demand that $f_{+}(0)=1$, i.e. we can multiply the left-hand-side by $Z$ to make this true. The temporal component of the vector current is the easiest to use for this purpose although the spatial component of the vector current is the one that we use for $J / \psi \rightarrow \eta_{c}$ decay. For a relativistic action such as HISQ the renormalisation of the spatial and temporal components will be the same up to discretisation errors.

For the 3 -point function needed to evaluate the matrix element above we use an NRQCD heavy quark propagating from 0 to $T$ and HISQ charm quarks from 0 to $t$ and $T$ to $t$ (see Fig. 5). The local staggered temporal vector current $\left(\gamma_{0} \otimes \gamma_{0}\right.$ in spin-taste notation) is inserted at $t$ and the restriction for staggered 3-point functions of an overall tasteless correlator is avoided by the spin content of the NRQCD propagator.

The 3-point function is given by:

$$
\begin{align*}
& C_{3 p t}(0, t, T)=\sum_{s_{T}, s_{t}}(-1)^{x_{T}+y_{T}+z_{T}+t_{T}}(-1)^{t_{t}}(\mathrm{~B}  \tag{B10}\\
& \times \operatorname{Tr}_{\mathrm{c}}\left\{g(t, T) \operatorname{Tr}_{\mathrm{s}}\left[\gamma_{0} \Omega^{\dagger}(T) G(T, 0) \Omega(0)\right] g^{\dagger}(t, 0)\right\}
\end{align*}
$$

The $g$ are HISQ $c$ propagators and $G$ is an NRQCD heavy quark propagator. The $\gamma_{0}$ factor comes from the local temporal vector current. The 3-point function is therefore calculated in a very similar way to the 2 -point function. $\Omega(x)$ multiplied by the random wall at the source time slice, 0 , is used as the source for the NRQCD propagator. At time T this is multiplied by $\Omega^{\dagger}$ and $\gamma_{0}$, source and sink spins are set equal and summed over. This is then the source for the HISQ propagator from $T$ to $t$ which is finally combined with the HISQ propagator generated from the random wall at time slice 0 .

We calculate the 2 -point and 3 -point functions described above for several different NRQCD masses, $m_{h} a$, and $c$ quark masses, $m_{c} a$, on the configuration sets 1,2 and 4 . We also use several different values of $T$ so that our fit benefits from both $T$ and $t$ dependence to improve the extraction of the ground-state masses, amplitudes and matrix elements. The 3 -point and 2 -point correlators are fit simultaneously to the forms given in eqs (1) and 25 . We use the same priors as in section III C. Note that for the 3 -point fit we can now impose symmetry under interchange of the mesons at 0 and $T$ since they are the same. This means that the amplitudes $V^{n n}$ and $V^{o o}$ are square symmetric matrices and $V^{n o}=V^{o n}$.

The key quantity that we extract from the fit is the ground state matrix element $V_{00}^{n n}$. This is proportional to the vector matrix element on the left-hand-side of eq. (B9). We can work out the constant of proportionality by matching our fit equations, eq (25) and (1) to the form expected by inserting a complete set of states in a continuum 3-point function. In this case factors of the mass of the meson ${ }^{4}$ cancel and we find $V_{00}^{n n}=f_{+}(0)$. Then the renormalisation factor we need is given by:

$$
\begin{equation*}
Z=\frac{1}{V_{00}^{n n}} \tag{B11}
\end{equation*}
$$

The results for $Z$ are taken from fits with 5 normal and 4 oscillating exponentials and given in Table IX. We obtain very precise results for $Z$, with errors of $0.1 \%$, without even using the full statistics available for each ensemble. The values are much more precise, for example, than for the implementation given in 53] (although their values are for light quarks rather than charm).

Figure 12 shows the quality of our results through plots of the ratio of the 3 -point to the 2 -point function. Note that we fit the 3 -point and 2 -point functions simultaneously and not just the ratio. It is convenient to plot the ratio, however, because the ground state contribution to this is simply $V_{00}^{n n}$. Our fit allows us to include the effect of excited states, both normal states and oscillating states. The presence of oscillating states is evident in the plots. The upper plot of Figure 12 compares results at different $T$ values. All are included in the simultaneous fit. The lower plot shows results at different values of $m_{h} a$ for a given $m_{c} a$.

The vector form factor method for determining $Z$ is completely nonperturbative. It will therefore be subject to errors coming from lattice QCD in the form of discretisation errors. These mean, for example, that the $Z$ factor at a particular value of the lattice spacing is not completely independent of the mass of the NRQCD spectator quark. From our results in Table IX we see that changing $m_{h} a$ from 2.8 to 1.5 on coarse set 2 (corresponding to change of almost a factor of two) causes a $2 \%$ change in $Z$. On fine set 4 the sensitivity is reduced to a change of $0.2 \%$, not significant within our statistical errors, when $m_{h} a$ is changed from 2.0 to 1.5 , a change in mass of $30 \%$. Since the change in lattice spacing between the coarse and fine sets is a factor of 1.4 , pairs of $a m_{h}$ values on coarse and fine lattices that correspond to approximately the same physical mass are $(2.8,2.0)$ and $(2.0,1.5)$. We will take our central result for $Z_{f f}$ from the $Z$ values corresponding to using $(2.0,1.5)$ and use $(2.8,2.0)$ to check systematic errors coming from $Z$. We see in section III C that we get the same answer from both sets of $Z$ values.

[^304]| Set $N_{\text {cfg }} \times N_{t} T$ | $a m_{h}$ | $a m_{c}$ | $\epsilon$ | $a E_{P_{c}}$ | $V_{00}^{n n}$ | $Z=Z_{f f}$ |  |  |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | $450 \times 4$ | 20,21 | 2.0 | 0.622 | -0.221 | $0.9630(2)$ | $1.0104(12)$ | $0.9896(11)$ |
| 2 | $408 \times 4$ | $20,21,24$ | 2.8 | 0.63 | -0.226 | $1.0239(2)$ | $1.0220(10)$ | $0.9784(9)$ |
|  |  | $20,21,24$ | 2.0 | 0.63 | -0.226 | $0.9719(2)$ | $1.0106(8)$ | $0.9894(8)$ |
|  |  | 20,21 | 1.5 | 0.63 | -0.226 | $0.9311(3)$ | $1.0026(14)$ | $0.9974(14)$ |
|  |  | 20,21 | 2.0 | 0.66 | -0.244 | $0.9994(3)$ | $1.0138(18)$ | $0.9863(17)$ |
| 4 | $322 \times 4$ | $24,25,30$ | 2.0 | 0.413 | -0.107 | $0.6454(2)$ | $0.9966(14)$ | $1.0033(14)$ |
|  |  | $24,25,30$ | 1.5 | 0.413 | -0.107 | $0.5939(2)$ | $0.9950(10)$ | $1.0049(10)$ |

TABLE IX: The $Z$ factors (column 9) obtained from the vector form factor method on different configurations sets (column 1) and for different NRQCD quark masses, $m_{h} a$ (column 4), and $c$ quark masses, $m_{c} a$ (column 5) with $\epsilon$ factor (column 6). The $m_{c} a$ values are those used in our calculation of $J / \psi \rightarrow \eta_{c} \gamma$ described in section III C; the $m_{h} a$ values are arbitrary since they correspond to the spectator quark. $Z$ is given by the inverse of the fit parameter $V_{00}^{n n}$ given in column 8. Column 2 gives the number of configurations used in the calculation and the number of time sources for the origin, 0 . The $T$ values used are given in column 3. Column 7 gives the energy of the NRQCD-c meson obtained from the fit. This is not equal to the mass because there is an energy offset in NRQCD.

| Set $m_{c} a$ | $a M_{\eta_{c}}$ | $\|a \vec{p}\|$ | $a E_{\eta_{c}}$ | $c^{2}$ |  |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 2 | 0.63 | $1.80851(4)$ | 0.52880 | $1.88286(12)$ | $0.9814(15)$ |
|  |  |  | 0.35000 | $1.84123(5)$ | $0.9748(5)$ |
|  |  |  | 0.20000 | $1.81923(4)$ | $0.9715(6)$ |
| 4 | 0.413 | $1.28042(4)$ | 0.37486 | $1.33352(6)$ | $0.9878(8)$ |
|  |  |  |  | 0.20000 | $1.29575(4)$ |
|  |  |  | $0.9873(7)$ |  |  |

TABLE X: Rest masses $\left(a M_{\eta_{c}}\right)$ and energies $\left(a E_{\eta_{c}}\right)$ at nonzero momentum $|a \vec{p}|$ for the Goldstone $\eta_{c}$ meson on sets 2 (coarse) and 4 (fine). The rest masses differ slightly from those in Table II because they come from independent fits; on set 4 we have higher statistics here. The zero and nonzero momentum correlator are fitted simultaneously and the speed of light, $c^{2}$, extracted using eq. (C1).

Table IX also shows results for the deliberately mistuned $c$ quark mass of 0.66 on set 2 with which we test the $c$ quark mass dependence of our $J / \psi \rightarrow \eta_{c}$ form factor. A barely significant change in $Z$ is seen between this value and that for the tuned mass of 0.63 . We also see no significant difference in $Z$ as we change the sea light quark masses between set 1 and set 2 .

Discretisation errors also mean that our results for $Z_{f f}$ here do not have to agree exactly with our earlier results for $Z_{c c}$. $Z_{c c}$ has a much larger error coming from unknown higher order terms in continuum perturbation theory. As a result of this, $Z_{f f}$ and $Z_{c c}$ do agree at the level of $1 \sigma$. They also agree within errors with the lattice QCD perturbation theory for this renormalisation, which has a small negative contribution at $\mathcal{O}\left(\alpha_{s}\right)$ 54.

The $Z$ values calculated here form part of a programme to normalise nonperturbatively a range of staggered currents for a variety of weak semileptonic and electromagnetic radiative decay rates 42].

## Appendix C: Discretisation errors

Finally we discuss discretisation errors. For relativistic formalisms the scale of discretisation errors can be set by the quark mass when this is larger than $\Lambda_{Q C D}$ and


FIG. 13: The 'speed-of-light', $c^{2}$, calculated from zero and finite momentum $\eta_{c}$ correlators using HISQ $c$ quarks. The top figure shows $c^{2}$ as a function of the square of the spatial momentum for coarse lattices, set 2 , where $m_{c} a=0.63$ (grey open circles) and for fine lattices, set 4 , where $m_{c} a=0.413$ (pink crosses). The lower figure shows the resulting values of $c^{2}$ as $\vec{p}^{2} a^{2} \rightarrow 0$ as a function of $\left(m_{c} a\right)^{2}$. The dashed straight line is drawn to guide the eye.


FIG. 14: The rest (static) and kinetic masses for the $\eta_{c}$ meson compared between the HISQ formalism (this paper) and the twisted mass formalism (Figure 3 from [10), and plotted against the square of the lattice spacing. The rest mass is given by open circles and the kinetic mass by open triangles, red for twisted mass and blue for HISQ. Errors include the full lattice spacing error on each point.


FIG. 15: $\quad R_{J / \psi}-1$ plotted against $a^{2}$ in $\mathrm{fm}^{2}$ for three different quark formalisms for the $c$ quark: HISQ (this paper, blue open circles), twisted mass (10], red open squares) and Fermilab clover ([29], green open triangles, showing results on the two finest lattices only). $R_{J / \psi}$ is $M_{J / \psi} / M_{\eta_{c}}$ so $R_{J / \psi}-1=\Delta M_{h y p} / M_{\eta_{c}}$. For the twisted mass and Fermilab clover results the heaviest and lightest sea quark masses are plotted at each value of the lattice spacing. Only statistical errors are shown. Additional errors from (twice) the lattice spacing error amount to $2 \%$ for HISQ and Fermilab clover and $4-7 \%$ for twisted mass. The black cross is the experimental average [7], offset slightly from the origin for clarity.


FIG. 16: $\quad f_{J / \psi}$ in GeV is plotted against $a^{2}$ in $\mathrm{fm}^{2}$ for the HISQ formalism (this paper, blue open circles) and for twisted mass ( 10 , red open squares). For the twisted mass case the heaviest and lightest sea quark masses are plotted at each value of the lattice spacing. Only statistical errors are shown for the twisted mass results. For the HISQ results we show the raw data from Table II with statistical and uncorrelated lattice spacing errors. There is an additional error of $1.3 \%$ from correlated lattice spacing and $Z$ factor uncertainties. The black cross is the experimental result from the average leptonic width [7], offset slightly from the origin for clarity.


FIG. 17: The vector form factor for $J / \psi \rightarrow \eta_{c}$ decay at $q^{2}=0, V(0)$, is plotted against $a^{2}$ in $\mathrm{fm}^{2}$ for the HISQ formalism (this paper, jpsigamma0 method, blue open circles) and for twisted mass ( 10 , red open squares). For the twisted mass case the heaviest and lightest sea quark masses are plotted at each value of the lattice spacing. Errors include statistical errors and uncertainties in the $Z$ factors. The black cross is the experimental result from the rate for $J / \psi \rightarrow \eta_{c} \gamma$ decay [26], offset slightly from the origin for clarity.
so they must be monitored closely when working with $c$ quarks.

One simple way to do this is through study of the energy of mesons at non-zero spatial momentum. Because the HISQ formalism is a relativistic formalism we determine meson masses as the result of fitting zeromomentum meson correlators as described in section II, For heavy quarks discretisation errors mean that this mass, known as the 'rest' or 'static' mass, can differ from the mass that controls the momentum-dependence of the energy at non-zero spatial momentum. This latter mass is known as the 'kinetic mass'. An equivalent statement is that the square of the speed-of-light, $c^{2}$, differs from 1 , where [11]

$$
\begin{equation*}
c^{2}(\vec{p})=\frac{E^{2}(\vec{p})-m^{2}}{\vec{p}^{2}} \tag{C1}
\end{equation*}
$$

For $\eta_{c}$ mesons we are able to determine $c^{2}$ very accurately with HISQ quarks when we have $\mathcal{O}(10,000)$ correlators as here. We fit zero and non-zero momentum simultaneously to the form given in eq. (1) (although the zero momentum correlators have no oscillating component). From the fit we obtain the ground state mass, $M_{0}$, in the zero momentum case and the ground state energy, $E_{0}$, in the non-zero momentum case. The simultaneous fit allows us to take correlations into account to improve the error in $c^{2}$. Results are given in Table X, $c^{2}$ is within $3 \%$ of 1 but we can distinguish it from 1 and we can see that it depends on the spatial momentum. This is shown in the top plot of Figure 13 for the coarse lattices, set 2, and the fine lattices, set 4. All tree-level $a^{2}$ errors are removed in HISQ but $c^{2}$ can depend linearly on $a^{2} \vec{p}^{2}$ through $\mathcal{O}\left(\alpha_{s}\right)$ corrections. We see that the slope of $c^{2}$ with $a^{2} \vec{p}^{2}$ is much smaller on the fine lattices than the coarse, as $m_{c} a$ is reduced. This plot can be compared with earlier results in Figure 9 of [55], although note that those results show a jump as the lattice momentum changes from $(1,1,1)$ to $(2,0,0)$. This results from a rotationally-noninvariant discretisation error not evident in our results because of the use of the phased boundary condition of eq. 16) to fix the momentum direction and simply change its magnitude.

From the top plot of Figure 13 we can determine the value of $c^{2}$ at $a^{2} \vec{p}^{2}=0$. The results from the coarse and fine lattices are then shown in the lower plot to lie on a straight line as a function of $\left(m_{c} a\right)^{2}$. The small slope is compatible with the $\left(m_{c} a\right)^{2}$ dependence also being an $\mathcal{O}\left(\alpha_{s}\right)$ effect. The straight line clearly goes through 1 as $m_{c} a \rightarrow 0$ as it must.

Another way to look at these discretisation errors is to compare the rest and kinetic masses for the $\eta_{c}$. The kinetic mass is given by 56]:

$$
\begin{equation*}
M_{k i n}=\frac{|\vec{p}|^{2}-(\Delta E)^{2}}{2 \Delta E} \tag{C2}
\end{equation*}
$$

where $\Delta E=E(\vec{p})-M_{\text {rest }}$. We also have $c^{2}=$ $M_{\text {rest }} / M_{k i n}$ 11. In the absence of errors, for a relativistic formalism, we should have $M_{\text {rest }}=M_{\text {kin }}$ (i.e. $c^{2}=1$ ).

In Figure 14 we compare the rest and kinetic masses for HISQ $\eta_{c}$ mesons using $M_{\text {kin }}=M_{\text {rest }} /\left(c^{2}\left(\vec{p}^{2}=0\right)\right)$ determined from Figure 13 . The rest and kinetic masses differ by $3 \%$ on the coarse lattices and $1.3 \%$ on the fine lattices.

Figure 14 also compares results from the twisted mass formalism, from [10]. For that formalism there is a significantly larger difference between rest and kinetic masses for the $\eta_{c}$ meson, amounting to $35 \%$ on the coarsest lattice spacing. The twisted mass formalism has tree-level $a^{2}$ errors, so a larger effect would be expected. The rest and kinetic masses agree in the continuum limit, as they must.

Figure 15 compares the hyperfine splitting in charmonium in units of the $\eta_{c}$ mass as a function of the square of the lattice spacing for the HISQ and twisted mass formalisms. The quantity plotted is $R_{J / \psi}-1$ where $R_{J / \psi}$ is defined in [10 as $M_{J / \psi} / M_{\eta_{c}}$ and results are given on each of their ensembles. The HISQ results are taken from Table II. We also show results from the Fermilab clover method [29] on their two finest sets of ensembles which correspond to the coarse and fine lattices used here.

All the results tend to the same continuum value which agrees with experiment. Much larger discretisation effects are visible for the twisted mass formalism than for HISQ. These are compatible with the tree level $a^{2}$ errors expected in that formalism, and with a mass scale of approximately 2 GeV (i.e. $m_{c}$ ). These tree level errors are removed in the HISQ formalism, but $\alpha_{s} a^{2}$ errors remain. These seem to be small for this quantity. The Fermilab clover discretisation errors, although in principle $\alpha_{s} a$, are also relatively small over this range of $a$.

Discretisation effects in the hyperfine splitting can also enter through tuning of the $c$ quark mass, because the hyperfine splitting is very sensitive to this. As discussed earlier in this section, there can be significant differences between rest and kinetic masses for mesons made of heavy quarks, and either can be used to tune the quark mass. Both relativistic formalisms, HISQ and twisted mass, use the rest mass. The Fermilab formalism uses the kinetic mass.

For $f_{J / \psi}$ the difference in discretisation effects between the HISQ and twisted mass formalisms is not as large. This is shown in Figure 16. Again, answers in agreement are obtained in the continuum limit. For the moments of the vector correlator our results for $G_{4}^{V}$ (Fig 4), which show very little dependence on the lattice spacing, can be compared to those for the twisted mass formalism in [57, where somewhat larger discretisation effects are visible.

Finally in Figure 17 we compare results for the vector form factor for $J / \psi \rightarrow \eta_{c}$ decay, $V(0)$. Large discretisation effects are evident in the twisted mass results. Once again discretisation effects in the HISQ results are small. Agreement in the continuum limit is again clear, however.

The HISQ results shown here give a further and more testing demonstration than that of [11, 36] of how small the discretisation errors for the HISQ action are, even for a quark as heavy as charm.
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# Direct determination of the strange and light quark condensates from full lattice QCD 

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#### Abstract

We determine the strange quark condensate from lattice QCD for the first time and compare its value to that of the light quark and chiral condensates. The results come from a direct calculation of the expectation value of the trace of the quark propagator followed by subtraction of the appropriate perturbative contribution, derived here, to convert the non-normal-ordered $m \bar{\psi} \psi$ to the $\overline{M S}$ scheme at a fixed scale. This is then a well-defined physical 'nonperturbative' condensate that can be used in the Operator Product Expansion of current-current correlators. The perturbative subtraction is calculated through $\mathcal{O}\left(\alpha_{s}\right)$ and estimates of higher order terms are included through fitting results at multiple lattice spacing values. The gluon field configurations used are 'second generation' ensembles from the MILC collaboration that include $2+1+1$ flavors of sea quarks implemented with the Highly Improved Staggered Quark action and including $u / d$ sea quarks down to physical masses. Our results are : $\langle\bar{s} s\rangle^{\overline{M S}}(2 \mathrm{GeV})=-(290(15) \mathrm{MeV})^{3},\langle\bar{l} l\rangle^{\overline{M S}}(2 \mathrm{GeV})=-(283(2) \mathrm{MeV})^{3}$, where $l$ is a light quark with mass equal to the average of the $u$ and $d$ quarks. The strange to light quark condensate ratio is $1.08(16)$. The light quark condensate is significantly larger than the chiral condensate in line with expectations from chiral analyses. We discuss the implications of these results for other calculations.


## I. INTRODUCTION

A critical feature of the nonperturbative dynamics of QCD at zero temperature is the condensation of quarkantiquark pairs in the vacuum, spontaneously breaking the chiral symmetry of the action. The value of the chiral condensate (the quark condensate at zero quark mass) is then an important parameter for low energy QCD [1]. The well-known Gell-Mann, Oakes, Renner (GMOR) relation [2]:

$$
\begin{equation*}
\frac{f_{\pi}^{2} M_{\pi}^{2}}{4}=-\frac{m_{u}+m_{d}}{2} \frac{\langle 0| \bar{u} u+\bar{d} d|0\rangle}{2} \tag{1}
\end{equation*}
$$

connects the $u / d$ quark masses times condensate to the square of the mass times decay constant for the Goldstone boson of the spontaneously broken symmetry. Eq.(11) has normalisation such that $f_{\pi}=130 \mathrm{MeV}$. The GMOR relation holds in the limit of $m_{u}, m_{d} \rightarrow 0$. A value for this chiral condensate can be derived from the chiral extrapolation of lattice QCD results for light meson masses and decay constants. See, for example, the recent result of $-(272(2) \mathrm{MeV})^{3}$ for the chiral condensate in the $\overline{M S}$ scheme at 2 GeV using $\mathrm{SU}(2)$ chiral perturbation theory 3 .

The determination of the quark condensate for nonzero quark masses is more problematic because, depending on the method used, there are various sources of un-

[^305]physical quark mass dependence and a careful definition of the condensate is required. This definition must be phrased in terms of the Operator Product Expansion (OPE) since this is the context in which the condensate appears [1, 4, 5]. The OPE allows us to separate short and long-distance contributions in, for example, a short-distance current-current correlator. The expansion is in terms of a set of matrix elements of local operators multiplied by coefficient functions. The aim is for all the long-distance contributions (with scale $<\mu$ ) to be contained in the matrix elements and the short distance contributions (with scale $>\mu$ ) in the coefficient functions. A key matrix element, since it corresponds to a relatively low-dimensional $(d=3)$ operator, is that of the quark condensate. The clean separation of scales in the OPE only works if the local operators are not normal ordered [6, 7]. Then the coefficient functions are analytic in the quark masses and therefore free of infrared sensitivity. This means, however, that the quark mass dependent mixing of $m \bar{\psi} \psi$ with the unit operator must be taken into account and that the vacuum matrix element of $m \bar{\psi} \psi$ is not cut-off independent. The quantity that appears in the OPE is the vacuum matrix element in, for example, the $\overline{M S}$ scheme at the scale $\mu$. We can derive this matrix element from lattice QCD and we give results here for $\mu=2 \mathrm{GeV}$. The results can easily be run to other scales, as appropriate.

The value of the condensate for quarks of non-zero mass up to that of the strange quark is needed in a number of calculations involving light quark correlators. In lattice QCD it is frequently easier and statistically more precise to use strange quarks than very light quarks in
contexts where the quark mass is not expected to be important. Then the strange quark condensate appears in the calculation, however. Examples include the matching to continuum QCD perturbation theory of lattice QCD calculations of moments of heavy-light meson correlators [8] and of light meson correlators at large space-like $q^{2}$ 9]. Such calculations are used to extract quark masses and the strong coupling constant, $\alpha_{s}$. A continuum example where the strange quark condensate is needed is in the determination of the strange quark mass, $m_{s}$, from hadronic $\tau$ decays [10].

Current estimates of the value of the strange quark condensate vary by almost a factor of two [11, 12]. It is not even clear whether the strange condensate is larger or smaller than the light quark condensate. For very large quark masses, $m_{q}>\Lambda_{Q C D}$, say, so that the quark mass dominates the propagator, it seems clear that the condensate should fall to zero, but this does not help in determining the slope of the condensate with $m_{q}$ for small quark masses.

Here we address the determination of the strange (or other non-zero mass) quark condensate by direct calculation in full lattice QCD. By direct we mean that we determine the vacuum expectation value of the strange quark propagator as well as the light quark propagator on a range of gluon field configurations at different values of the lattice spacing and sea quark masses. To isolate the low-energy nonperturbative value of the condensate from these results requires the subtraction of a perturbative contribution. The perturbative contribution in lattice QCD has two pieces. One diverges as $a \rightarrow 0$ and dominates the vacuum expectation value of the strange quark propagator, particularly on our finer lattices. The second piece contains infrared sensitive logarithms of the quark mass which cancel against similar terms in continuum perturbation theory allowing an infrared safe definition of the condensate for use in the OPE, as discussed above.

The error in the final result then depends on how well this subtraction can be done. Here we use an explicit calculation of the perturbative pieces through $\mathcal{O}\left(\alpha_{s}\right)$ and fit for unknown higher order terms. The known quark mass and $a$ dependence of these unknown terms helps in constraining them along with the very small statistical errors in our lattice results. We also use a particularly good discretisation of the Dirac action known as the Highly Improved Staggered Quark (HISQ) formalism [13] on 'second generation' gluon field configurations so that discretisation errors in the physical nonperturbative results are small.

The paper is laid out as follows. In Section II we describe the theoretical background to direct calculations of the quark condensate in lattice QCD. Section III gives our lattice QCD results on gluon configurations with $2+1+1$ flavors of sea quarks, describing the calculation of the perturbative contribution that is subtracted and then the procedure for fitting the remaining nonperturbative condensates as a function of quark mass and lattice
spacing. We also give results from configurations including $2+1$ flavors of sea quarks over a wider range of lattice spacing values but studying only the strange quark condensate in Appendix D. In Section IV we compare to previous values and discuss the implications of our results for both zero and finite temperature QCD calculations. Section V gives our conclusions.

## II. THEORETICAL BACKGROUND

The direct determination of the chiral condensate in lattice QCD requires the calculation of the expectation value over an ensemble of gluon fields, $U$, of $\operatorname{Tr} M^{-1}$ where $M$ is the lattice discretisation of the Dirac matrix. The quark action for a given quark flavor,

$$
\begin{equation*}
S_{f}=\bar{\psi} M_{f} \psi \tag{2}
\end{equation*}
$$

and

$$
\begin{equation*}
\langle\bar{\psi} \psi\rangle=\langle 0| \bar{\psi}_{f} \psi_{f}|0\rangle=-\frac{1}{V}\left\langle\operatorname{Tr} M_{f}(U)^{-1}\right\rangle_{U} \tag{3}
\end{equation*}
$$

where the trace is over spin, color and space-time point and the gluon fields in the ensemble used for the average include the effect of sea quarks (of all flavors, not just $f$ ) in their probability distribution. $V$ is the lattice volume, $L^{3} \times T$. For a naive discretisation of the Dirac action $M$ takes the form:

$$
\begin{equation*}
M=\gamma_{\mu} \Delta_{\mu}+m \tag{4}
\end{equation*}
$$

where $\Delta_{\mu}$ is a covariant finite difference on the lattice:

$$
\begin{equation*}
\Delta_{\mu} \psi_{x}=\frac{1}{2 a}\left(U_{\mu}(x) \psi(x+\hat{\mu})-U_{\mu}^{\dagger}(x-\hat{\mu}) \psi(x-\hat{\mu})\right) \tag{5}
\end{equation*}
$$

and $m$ is the quark mass for that flavor. Because of fermion doubling this formalism describes 16 'tastes' of quarks in 4-dimensions rather than just 1 and we must divide the right-hand side of Eq. (3) by the number of tastes, $N_{t}=16$. The staggered formalism is derived from this naive formalism by a rotation which allows the spin degree of freedom to be dropped. In that case the quark field becomes a 1-component spinor, which is numerically very efficient, and $N_{t}=4$.

For $m=0$ the eigenvalues of $M$ for either naive or staggered quarks, are purely imaginary and come in $\pm$ pairs. Therefore, in the absence of exact zero modes,

$$
\begin{align*}
-\langle\bar{\psi} \psi\rangle & =\frac{1}{N_{t}} \sum_{\lambda}\left(\frac{1}{m+i \lambda}+\frac{1}{m-i \lambda}\right) \\
& =\frac{1}{N_{t}} \sum_{\lambda} \frac{2 m}{m^{2}+\lambda^{2}} \tag{6}
\end{align*}
$$

A calculation at $m=0$ on a finite volume lattice would then give an answer for the quark condensate of zero. This does not mean that chiral symmetry is unbroken,
however. The problem arises because the broad distribution of non-zero eigenvalues (ignoring topological nearzero modes) drops to zero near the origin in a way that depends strongly on the volume. Once the quark mass is below the minimum of the non-zero eigenvalues the result for $\langle\bar{\psi} \psi\rangle$ will be distorted. A more careful consideration of limits must be made. If $V$ is taken to infinity before $m$ is taken to zero then the sum over eigenvalues can be replaced by an integral and the Banks-Casher relation 14 is obtained. This connects the zero-mass condensate to the spectral density at the origin:

$$
\begin{equation*}
\Sigma=-\langle\bar{\psi} \psi(m=0)\rangle=\frac{\pi \rho(0)}{N_{t}} \tag{7}
\end{equation*}
$$

Thus $\Sigma$ can be obtained from studies of the spectral density and, more recently, has also been obtained from matching the distribution of low eigenmodes to random matrix theory in the $\epsilon$ regime [15-17]. Here we are more concerned with extracting a condensate at nonzero quark mass, for example at the strange quark mass, and so the issue above is not relevant. We will work on large volume lattices (over ten times larger than the study in [18] that looked at staggered eigenvalues in the $\epsilon$ regime) at quark mass values that are well within the distribution of non-zero eigenvalues. Our results for $\left\langle\operatorname{Tr} M^{-1}\right\rangle$ then include both the effects of a non-zero value for $\rho(0)$ and a non-zero quark mass.

A second issue arises, however, in the extraction of a physical nonperturbative value for the condensate at non-zero quark mass. A perturbative contribution appears from mixing between the scalar $\bar{\psi} \psi$ operator and the identity since the identity operator has a vacuum expectation value in the trivial perturbative vacuum. This perturbative contribution vanishes at zero quark mass since chiral symmetry is not broken in perturbation theory (for the same reason as that given on the lattice above in Eq. (6)). At non-zero quark mass it contains odd powers of $m$ starting with a quadratically ultra-violet divergent term linear in $m$. This can be illustrated with a tree-level calculation in the continuum to give:

$$
\begin{align*}
-\langle\bar{\psi} \psi\rangle & =\int_{0}^{\Lambda} \frac{d^{4} k}{(2 \pi)^{4}} \frac{12 m}{k^{2}+m^{2}}  \tag{8}\\
& =\frac{3}{4 \pi^{2}}\left(m \Lambda^{2}+m^{3} \log \frac{m^{2}}{\Lambda^{2}+m^{2}}\right)
\end{align*}
$$

The quadratic ultraviolet divergence depends on the scheme used but the $m^{3} \log (m / \Lambda)$ term is universal since it arises from the infrared part of the integral. The coefficient above agrees with that obtained for the $\overline{M S}$ scheme in [19] and on the lattice for highly improved staggered quarks to be described in section IIIA. We stress that a perturbative contribution of this kind is present for all lattice regularisations of QCD, whatever their chiral symmetry properties, and so must be calculated and subtracted to give a physical result. The quadratic divergence present for Ginsparg-Wilson fermions is demonstrated in the quenched approximation in, for exam-
ple, 20 and the additional divergences for the Wilson formalism with broken chiral symmetry in 21].

This subtraction is somewhat analogous to subtracting perturbative contributions to the mean plaquette to obtain the nonperturbative gluon condensate. That, however, is extremely difficult to do because the nonperturbative condensate contribution to the plaquette is so small. This contribution is given at leading order by:

$$
\begin{equation*}
\delta P_{c o n d}=-\frac{\pi^{2}}{36} a^{4}\left\langle\alpha_{s} G^{2} / \pi\right\rangle \tag{9}
\end{equation*}
$$

If we take the value of the gluon condensate as $\mathcal{O}\left(\Lambda_{Q C D}^{4}\right)$ then $\left\langle\alpha_{s} G^{2} / \pi\right\rangle \approx 0.005 \mathrm{GeV}^{4}$. On very coarse lattices for which $a \approx 1 \mathrm{GeV}^{-1}$, this contributes less than $1 \%$ to the value of the plaquette. On finer lattices the nonperturbative condensate contribution is even smaller because it falls as $a^{4}$ while the perturbative contribution falls only as $\alpha_{s}(d / a)$ for some scale $d$. This means that the plaquette is in fact a very good variable to use for the determination of $\alpha_{s}$ from lattice QCD calculations but not for the determination of the gluon condensate [22]. For larger Wilson loops the gluon condensate contribution is larger, being proportional to the square of the area of the loop, but the coefficients in the perturbative series also become larger.

The determination of the nonperturbative quark condensate from $\left\langle\operatorname{Tr} M^{-1}\right\rangle$ is in much better shape than this for several reasons. The main one is that the nonperturbative condensate contribution to $\left\langle\operatorname{Tr} M^{-1}\right\rangle$ in lattice units is only a factor of $a^{2}$ smaller than the leading perturbative contribution rather than $a^{4}$. In addition the perturbative contribution is suppressed by the quark mass, which is small for the $u / d$ and $s$ quarks we will consider here. The perturbative contribution is a welldefined function of the quark mass at every order in perturbation theory and so results at several values of the quark mass, and the lattice spacing, can be used to constrain unknown higher orders, beyond the $\mathcal{O}\left(\alpha_{s}\right)$ that we have explicitly calculated, and we will make use of that here.

## III. LATTICE QCD CALCULATION ON $n_{f}=2+1+1$ GLUON CONFIGURATIONS

The gluon field configurations used here are listed in Table They were generated by the MILC collaboration [23] using a tadpole-improved Lüscher-Weisz gauge action with coefficients corrected perturbatively through $\mathcal{O}\left(\alpha_{s}\right)$ including pieces proportional to $n_{f}$, the number of quark flavors in the sea [24]. The gauge action is then improved completely through $\mathcal{O}\left(\alpha_{s} a^{2}\right)$. Sea quarks are included with the highly improved staggered quark (HISQ) action [13] which has been designed to have very small discretisation errors. Discretisation errors are formally removed through $\mathcal{O}\left(a^{2}\right)$ but higher order errors, particularly staggered taste-changing errors, are seen to

TABLE I: Details of the MILC gluon field ensembles used in this paper. $\beta=10 / g^{2}$ is the $S U(3)$ gauge coupling and $L / a$ and $T / a$ are the number of lattice spacings in the space and time directions for each lattice. $a m_{l, \text { sea }}, a m_{s, \text { sea }}$ and $a m_{c, \text { sea }}$ are the light (up and down taken to have the same mass), strange and charm sea quark masses in lattice units. $a$ is the lattice spacing in fm determined from the decay constant of the $\eta_{s}$ meson in [25] with values for 3,6 and 8 added here. The ensembles 1,2 and 3 will be referred to in the text as "very coarse", 4,5 and 6 as "coarse" and 7 and 8 as "fine."

| Set | $\beta$ | $a / \mathrm{fm}$ | $a m_{l, \text { sea }}$ | $a m_{s, \text { sea }}$ | $a m_{c, \text { sea }}$ | $L / a \times T / a$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 5.80 | $0.1546(11)$ | 0.013 | 0.065 | 0.838 | $16 \times 48$ |
| 2 | 5.80 | $0.1526(8)$ | 0.0064 | 0.064 | 0.828 | $24 \times 48$ |
| 3 | 5.80 | $0.1511(8)$ | 0.00235 | 0.0647 | 0.831 | $32 \times 48$ |
| 4 | 6.00 | $0.1234(8)$ | 0.0102 | 0.0509 | 0.635 | $24 \times 64$ |
| 5 | 6.00 | $0.1218(6)$ | 0.00507 | 0.0507 | 0.628 | $32 \times 64$ |
| 6 | 6.00 | $0.1206(6)$ | 0.00184 | 0.0507 | 0.628 | $48 \times 64$ |
| 7 | 6.30 | $0.0899(7)$ | 0.0074 | 0.0370 | 0.440 | $32 \times 96$ |
| 8 | 6.30 | $0.0875(7)$ | 0.0012 | 0.0363 | 0.432 | $64 \times 96$ |

be smaller with HISQ than with the earlier asqtad staggered quark action [13, 23]. The HISQ action used here has two smearing steps for the gluon field appearing in the quark action with a $\mathrm{U}(3)$ projection of the smeared links between the two smearing steps. The configurations include a sea charm quark in addition to up, down and strange. These configurations are then said to have $2+1+1$ flavors in the sea, since the $u$ and $d$ quarks are taken to have the same mass (denoted $m_{l}$ here). This is heavier than the average $u / d$ mass in the real world on most of the configuration sets but there are three for which the $u / d$ mass has its physical value ( 3,6 and 8 ). The $s$ and $c$ masses are tuned as closely as possible to their correct values on each set. The tuning of the sea $s$ quark mass is accurately done - typically to better than $5 \%$ - so the $u / d$ quark mass can be accurately calibrated in terms of the $s$ quark mass for chiral extrapolations. The values of the lattice spacing for most ensembles were determined in [25] using the decay constant of the $\eta_{s}$ meson. The values vary from 0.15 fm to 0.09 fm as we go from the very coarse to the fine lattices. The spatial volumes are large, from $(2.5 \mathrm{fm})^{3}$ when $m_{l} / m_{s} \approx 0.2$ to $(3.7 \mathrm{fm})^{3}$ when $m_{l} / m_{s} \approx 0.1$.

On each of these ensembles we determine $\left\langle\operatorname{Tr} M^{-1}\right\rangle$ for HISQ valence quarks for various quark masses. To do this we use an identity that relates the quark propagator for staggered quarks to a product of quark propagators:

$$
\begin{align*}
\frac{1}{a m_{q}} \operatorname{Tr} M_{00}^{-1} & =\sum_{n} \operatorname{Tr}\left[M_{0 n}^{-1} M_{n 0}^{-1}\right](-1)^{n} \\
& =\sum_{n} \operatorname{Tr}\left|M_{0 n}^{-1}\right|^{2} \tag{10}
\end{align*}
$$

Here 0 and $n$ are arbitrary lattice sites and $a m_{q}$ is the quark mass in lattice units used for the quark propagator. The righthand side of Eq. 10 is simply the correlator between 0 and $n$ for the Goldstone pseudoscalar meson


FIG. 1: Autocorrelation function, $C_{\Delta T}$ of Eq. 12 for the strange and light quark condensates on coarse set 6 with physical mass light sea quarks. The $x$-axis, $\Delta T$, is the separation in time units between configurations. The strange condensate results are given as blue crosses and the light condensate with red pluses. Errors in $C_{\Delta T}$ are estimated by dividing the configuration time series into five consecutive sets.
made of a quark and antiquark of mass $a m_{q}$. Summing over $n$ projects on to zero spatial momentum and sums over timeslices. Thus, dividing both sides by 4 , the number of tastes for staggered quarks, we obtain:

$$
\begin{equation*}
-a^{3}\langle\bar{\psi} \psi\rangle_{0}=\left(a m_{q}\right) \sum_{t} C_{\pi}(t) \tag{11}
\end{equation*}
$$

The raw condensate value on the left-hand side of this expression is normalised to the single flavor case and the pion correlator on the right-hand side is the usual zeromomentum Goldstone meson correlator. This allows us to determine $\langle\bar{\psi} \psi\rangle_{0}$ by summing over the Goldstone pseudoscalar correlators calculated in [25]. Eq. (10) is derived in [26] for a single propagator origin, 0 , but the derivation can trivially be extended to hold for the random wall source that we use for our correlators in [25]. The identity holds configuration by configuration for lattice QCD quark formalisms with sufficient chiral symmetry and in the continuum for a specific gauge field background. We give an explicit proof of this in Appendix A. Since our Goldstone pseudoscalar correlators are sums of positive numbers they are particularly precise and this precision then carries over to our condensate results. For the light condensate we use the pion correlators made of light quarks and for the strange condensate we use the $\eta_{s}$ correlators made of strange quarks. We stress that what we calculate using Eq. 10 is the vacuum expectation value of the condensate (and not a specific 'in-meson' value) despite the fact that we determine it for convenience from a meson correlator.

Table $\Pi$ gives the valence quark masses used in our calculation and the raw results for the condensate obtained from Eq. 10). The correlator calculations used 16 'random wall' time sources on approximately one thousand

TABLE II: Raw (unsubtracted) values for the light and strange quark condensates in lattice units calculated for valence masses given in columns 2 and 3. The results use the correlators calculated in 25 (via Eq. (11) , but we also give results for additional strange quark masses on sets 1 and 2 and new results on sets 3,6 and 8 . We have 16,000 correlators per ensemble, except for sets 6 and 8 where we use approximately 10000 .

| Set | $a m_{l, v a l}$ | $a M_{\pi}$ | $a f_{\pi}$ | $-a^{3}\left\langle\bar{\psi} \psi_{l}\right\rangle_{0}$ | $a m_{s, v a l}$ | $a M_{\eta_{s}}$ | $a f_{\eta_{s}}$ | $-a^{3}\left\langle\bar{\psi} \psi_{s}\right\rangle_{0}$ |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 0.013 | $0.23637(15)$ | $0.11183(9)$ | $0.018607(29)$ | 0.0688 | $0.53361(14)$ | $0.14199(6)$ | $0.045758(19)$ |
|  |  |  |  |  |  | 0.0641 | $0.51491(14)$ | $0.13996(6)$ |
| 2 | 0.0064 | $0.16615(7)$ | $0.10511(5)$ | $0.014524(18)$ | 0.0679 | $0.52797(8)$ | $0.14026(3)$ | $0.045616(19)$ |
|  |  |  |  |  | 0.0636 | $0.51078(8)$ | $0.13839(3)$ | $0.043038(12)$ |
| 3 | 0.00235 | $0.10172(5)$ | $0.09934(5)$ | $0.011762(11)$ | 0.0628 | $0.50657(5)$ | $0.13720(3)$ | $0.042483(6)$ |
| 4 | 0.01044 | $0.19153(9)$ | $0.09075(5)$ | $0.011629(13)$ | 0.0522 | $0.42351(9)$ | $0.11312(4)$ | $0.031756(10)$ |
| 5 | 0.00507 | $0.13413(5)$ | $0.08451(4)$ | $0.008511(9)$ | 0.0505 | $0.41476(6)$ | $0.11119(2)$ | $0.030768(6)$ |
| 6 | 0.00184 | $0.08154(2)$ | $0.07988(2)$ | $0.006534(6)$ | 0.0507 | $0.41481(2)$ | $0.11062(2)$ | $0.030768(4)$ |
| 7 | 0.0074 | $0.14070(9)$ | $0.06621(5)$ | $0.006153(8)$ | 0.0364 | $0.30884(11)$ | $0.08238(4)$ | $0.019822(4)$ |
| 8 | 0.0012 | $0.05718(2)$ | $0.05781(3)$ | $0.002803(4)$ | 0.0360 | $0.30483(4)$ | $0.08055(2)$ | $0.019504(2)$ |

configurations in each ensemble (somewhat fewer on sets 6 and 8$)$ and so the results have very small statistical errors. The valence light quark masses are equal to those in sea (except for a very small change on set 3 ) but we have shifted the valence strange quark masses slightly to be closer to the physical strange quark mass, following [25]. On sets 1 and 2 we give results for two different values of the strange quark mass, to help in constraining the valence mass dependence of the condensate.

Errors on the condensate values are determined after binning over adjacent sets of at least five configurations, following analysis of the autocorrelation function. An example plot is shown, for coarse set 6, in Fig. 1. The autocorrelation function is defined as:

$$
\begin{equation*}
C_{\Delta T}=\frac{\left\langle x_{i} x_{i+\Delta T}\right\rangle-\left\langle x_{i}\right\rangle\left\langle x_{i+\Delta T}\right\rangle}{\left\langle x_{i}^{2}\right\rangle-\left\langle x_{i}\right\rangle^{2}} . \tag{12}
\end{equation*}
$$

Here $x_{i}$ represents a condensate value on configuration $i$ and $x_{i+\Delta T}$ that on a configuration a further $\Delta T$ time units along in the ordered ensemble. $\Delta T=1$ thus corresponds to adjacent configurations. Fig. 1 shows that nearby configurations in the ensembles are correlated and thus binning is necessary to obtain a reliable statistical error. A similar analysis applies to masses and decay constants as discussed in 25].

In the next section we describe the perturbative calculation of the condensate which we will then subtract from the raw results of Table II to enable the nonperturbative condensate to be determined.

## A. Perturbative calculation of $\left\langle\operatorname{Tr} M^{-1}\right\rangle$

We computed the perturbative contribution $\langle\bar{\psi} \psi\rangle_{\mathrm{PT}}$ to the chiral condensate for the HISQ action through firstorder in $\alpha_{s}$ :

$$
\begin{aligned}
-a^{3}\langle\bar{\psi} \psi\rangle_{\mathrm{PT}, \mathrm{HISQ}}= & a m_{0} \times \\
& {\left[c_{0}\left(a m_{0}\right)+c_{1}\left(a m_{0}\right) \alpha_{s}+O\left(\alpha_{s}^{2}\right)\right] }
\end{aligned}
$$

where $a m_{0}$ is the bare quark mass parameter that appears in the HISQ action. The Feynman diagrams required to this order are shown in Fig. 2. The perturbative quadratic ultraviolet divergence discussed in eq. (9) shows up as finite values for the perturbative coefficients, as defined above, in the limit $a m_{0} \rightarrow 0$.


FIG. 2: Feynman diagrams for the calculation of the perturbative contribution to the quark condensate through $\mathcal{O}\left(\alpha_{s}\right)$.

We computed the coefficients from numerical evaluation of the lattice loop integrals over a range of masses that includes the light and strange quark masses that we have used. A representative sample of our results is given in Table III, and is illustrated in Fig. 3 .

An excellent fit to the perturbative coefficients in this range of small quark masses, $a m_{0} \lesssim 0.1$, can be obtained using the following parameterizations

$$
\begin{equation*}
c_{0}\left(a m_{0}\right)=c_{00}+\left(a m_{0}\right)^{2}\left[c_{01} \log \left(a m_{0}\right)+c_{02}\right] \tag{14}
\end{equation*}
$$

and

$$
\begin{align*}
c_{1}\left(a m_{0}\right)= & c_{10}+\left(a m_{0}\right)^{2}\left[c_{11} \log ^{2}\left(a m_{0}\right)\right. \\
& \left.+c_{12} \log \left(a m_{0}\right)+c_{13}\right] . \tag{15}
\end{align*}
$$

Higher order terms in $a m_{0}$ appear as discretisation errors in the comparison to $\overline{M S}$ to be done below and so can be ignored - they are negligible for the masses we are using in any case. The leading logarithm of $a m_{0}$ at each order originates entirely from the infrared region of the
loop momenta, and the respective coefficients $c_{01}$ and $c_{11}$ can easily be computed analytically. The values of these coefficients must and do agree with the values in the $\overline{M S}$ scheme [19]. At one-loop we also have a constraint on the sub-leading (single) logarithm of $a m_{0}$ since, as discussed in Appendix C, all $\log m$ terms must vanish in the difference between the vacuum expectation values of $m \bar{\psi} \psi$ in perturbation theory in the continuum and on the lattice. Allowing for the renormalisation between the $\overline{M S}$ mass and the HISQ bare mass:

$$
\begin{equation*}
\bar{m}(\mu)=m_{0}\left(1+\alpha_{s}\left[-\frac{2}{\pi} \log a \mu+0.1143(3)\right]+\ldots\right) \tag{16}
\end{equation*}
$$

we find that $c_{12}$ should have the value $0.2307(2)$. With the logarithmic terms fixed to their known values we can obtain the other coefficients in eqs. (14) and 15 from a fit to the values for $c_{0}\left(a m_{0}\right)$ and $c_{1}\left(a m_{0}\right)$ as a function of $a m_{0}$. We find:

$$
\begin{align*}
& c_{00}=0.38366(1) \\
& c_{01}=3 /\left(2 \pi^{2}\right) \\
& c_{02}=-0.153(1) \tag{17}
\end{align*}
$$

and

$$
\begin{align*}
& c_{10}=0.03657(7) \\
& c_{11}=-6 / \pi^{3} \\
& c_{12}=0.2307(2) \\
& c_{13}=0.308(15) \tag{18}
\end{align*}
$$

These fits are illustrated in Fig. 3 and reproduce our results for the coefficients to within their numerical integration errors, which are smaller than about $0.01 \%$ for $c_{0}$, and $1 \%$ for $c_{1}$.

The perturbative determination of the vacuum expectation value of $\bar{\psi} \psi$ has also been done in the $\overline{M S}$ scheme, in [19]. The power divergence is missing in this case but, as discussed above, there are terms proportional to $m^{3} \log m$. 19] finds:

$$
\begin{align*}
- & \langle\bar{\psi} \psi\rangle_{\mathrm{PT}, \mathrm{MS}}^{(\mu)}=\bar{m}^{3}(\mu) \times  \tag{19}\\
& {\left[d_{01} l_{m}+d_{02}+\alpha_{s}\left(d_{11} l_{m}^{2}+d_{12} l_{m}+d_{13}\right)+\ldots\right] }
\end{align*}
$$

where $l_{m}=\log (\bar{m}(\mu) / \mu)$ and

$$
\begin{align*}
d_{01} & =c_{01}=\frac{3}{2 \pi^{2}} \\
d_{02} & =-\frac{3}{4 \pi^{2}} \\
d_{11} & =c_{11}=-\frac{6}{\pi^{3}} \\
d_{12} & =\frac{5}{\pi^{3}} \\
d_{13} & =-\frac{5}{2 \pi^{3}} \tag{20}
\end{align*}
$$

TABLE III: Zeroth- and first-order coefficients, $c_{0}$ and $c_{1}$ respectively, for the perturbative condensate, Eq. 14 , for representative values of the bare quark mass parameter $a m_{0}$ in lattice units. The uncertainties are from a numerical evaluation of the lattice perturbation theory loop integrals.

| $a m_{0}$ | $c_{0}$ | $c_{1}$ |
| :--- | :---: | :---: |
| 0.088 | $0.37962(2)$ | $0.02561(12)$ |
| 0.079 | $0.38029(1)$ | $0.02709(13)$ |
| 0.0728 | $0.38075(1)$ | $0.02793(16)$ |
| 0.067 | $0.38113(1)$ | $0.02902(18)$ |
| 0.062 | $0.38146(1)$ | $0.02963(14)$ |
| 0.0564 | $0.38178(1)$ | $0.03049(22)$ |
| 0.0505 | $0.38212(1)$ | $0.03139(16)$ |
| 0.0448 | $0.38240(1)$ | $0.03203(18)$ |
| 0.0386 | $0.38271(1)$ | $0.03267(20)$ |
| 0.032 | $0.38296(1)$ | $0.03349(24)$ |
| 0.028 | $0.38313(1)$ | $0.03421(21)$ |
| 0.024 | $0.38325(1)$ | $0.03424(21)$ |
| 0.020 | $0.38336(1)$ | $0.03548(26)$ |
| 0.016 | $0.38347(2)$ | $0.03545(34)$ |
| 0.01044 | $0.38356(1)$ | $0.03614(49)$ |
| 0.00507 | $0.38364(2)$ | $0.03631(31)$ |

As discussed in Appendix B we must subtract the difference between the lattice QCD and $\overline{M S}$ perturbative calculations from our lattice QCD results to obtain the nonperturbative condensate in the $\overline{M S}$ scheme at the scale $\mu$. We work with the combination $m \bar{\psi} \psi$ which would be RG-invariant in the absence of this perturbative contribution and it is convenient to derive the subtraction needed in lattice units and as a function of the bare lattice quark mass. Using eq. 166 we obtain

$$
\begin{align*}
\Delta_{\mathrm{PT}} & =-a^{4}\left(\left\langle m_{0} \bar{\psi} \psi\right\rangle_{\mathrm{PT}, \mathrm{HISQ}}-\langle\bar{m}(\mu) \bar{\psi} \psi\rangle_{\mathrm{PT}, \overline{\mathrm{MS}}}\right) \\
& =c_{00}\left(a m_{0}\right)^{2}+\alpha_{s} c_{10}\left(a m_{0}\right)^{2}  \tag{21}\\
& +\left(a m_{0}\right)^{4}\left[c_{01} l_{\mu}-0.077(1)\right] \\
& +\alpha_{s}\left(a m_{0}\right)^{4}\left[c_{11} l_{\mu}^{2}+0.1340(2) l_{\mu}+0.406(15)\right]+\ldots
\end{align*}
$$

where $l_{\mu}=\log (\mu a)$. This difference of perturbative expansions is now free of all logarithms of $m$ and therefore well-defined and infrared safe.

## B. Determining the nonperturbative strange and

 light quark condensates
## 1. A first look at the results

The physical condensate in the $\overline{M S}$ scheme at the scale $\mu$ is then defined by:

$$
\begin{equation*}
\langle m \bar{\psi} \psi\rangle_{N P, \overline{M S}}(\mu)=a^{-4}\left(a^{4}\langle m \bar{\psi} \psi\rangle_{0}-\Delta_{P T}\right) \tag{22}
\end{equation*}
$$

where $\langle m \bar{\psi} \psi\rangle_{0}$ is the numerical result from lattice QCD and $\Delta_{P T}$ is given through $\mathcal{O}\left(\alpha_{s}\right)$ as a function of the quark mass in Eq. 21. $\Delta_{P T}$ will also contain unknown


FIG. 3: Zeroth- and first-order coefficients, $c_{0}$ and $c_{1}$ respectively, for the perturbative condensate, Eq. (14), versus the bare quark mass parameter $a m_{0}$ in lattice units. The uncertainties in $c_{0}$ resulting from numerical evaluations of the lattice loop integral are not visible in that plot. The fits given in the text are plotted as dashed lines.
higher order pieces in $\alpha_{s}$ that we can try to determine from a fit to the lattice QCD results. First we look at the effect of the calculated tree-level and one-loop contributions.
$\Delta_{P T}$ is a strong function of the quark mass in lattice units, dominated by the $(m a)^{2}$ terms that give rise to the quadrative divergence with inverse lattice spacing. This means that the relative size of the subtraction compared to the raw results varies strongly with quark mass and with lattice spacing, and this is reflected in the raw results before the subtraction is made. In Fig. 4 the open squares show the unsubtracted results (i.e. setting $\Delta_{P T}$ to zero in Eq. (22p) as a function of the square of the inverse lattice spacing for quarks at the four different masses that we have results for in Table II. strange quarks and light quarks of masses $m_{s} / 5$ (sets 1,4 and 7 ), $m_{s} / 10$ (sets 2 and 5) and the physical value, $m_{s} / 27$ (sets 3, 6 and 8 ).

Instead of plotting the condensate results directly, the
$y$-axis in Fig. 4 is:

$$
\begin{equation*}
R_{l}=-\frac{4 m_{l}\left\langle\bar{\psi} \psi_{l}\right\rangle}{\left(f_{\pi}^{2} M_{\pi}^{2}\right)} \tag{23}
\end{equation*}
$$

for light quarks and

$$
\begin{equation*}
R_{s}=-\frac{4 m_{s}\left\langle\bar{\psi} \psi_{s}\right\rangle}{\left(f_{\eta_{s}}^{2} M_{\eta_{s}}^{2}\right)} \tag{24}
\end{equation*}
$$

for strange quarks. The values of the raw unsubtracted $R_{q}$ are determined directly from Table II using the $a m$, $a M, a f$ and $\langle\bar{\psi} \psi\rangle_{0}$ values given there.

The ratio $R_{q}$ is a good quantity to plot (and later to use in our fits) for a number of reasons:

- $m\langle\bar{\psi} \psi\rangle$ is a physical renormalisation-group invariant quantity as $m \rightarrow 0$, up to discretisation errors, as is clear from the GMOR relation. The division by the square of the meson decay constant times its mass makes a dimensionless ratio which is convenient but it is also one that (from the GMOR relation) we expect to be close to 1 .
- Using the ratio $R_{q}$ also reduces the effect of any slight mistuning of quark masses since the quark mass multiplied in the numerator cancels against the square of the meson mass in the denominator. The tuning of $m_{s}$ uses the $\eta_{s}$ decay constant, as described in 25]. This means that, by definition, $f_{\eta_{s}}$ does not contain discretisation errors that would mask the identification of the pieces that diverge as $a \rightarrow 0$.
- Finally the ratio has reduced finite-volume effects over that in either the numerator or denominator. This is expected from the fact that chiral loop effects, which are sensitive to the volume, cancel in $R_{q}$ [27, [28]. This is illustrated in Fig. 5 where we show results [29] for pion mass, decay constant and (unsubtracted) light quark condensate as well as the ratio $R_{l}$ of Eq. (23) for ensembles with $a m_{l, \text { sea }}=0.00507$ and $a m_{s, \text { sea }}=0.0507$ and three different spatial volumes. The spatial volumes correspond to a spatial length in lattice units of 24,32 and 40. The set with $L / a=32$ is our set 4 (see Table $\bar{I}$. For each quantity we plot the ratio of the value at $L / a$ to that at $L / a=40$. It is clear from the plot that the finite volume dependence in each of $m_{\pi}, f_{\pi}$ and $\langle\bar{\psi} \psi\rangle_{l}$ is cancelled to a very high level of accuracy ( $0.1(1) \%$ for set 4) in $R_{l}$.

Figure 4 shows clearly the presence of a quadratic divergence with $a^{-2}$ in the raw results. This is very 'clean' in our calculations because the form of the divergence is very constrained. Only a term of the form $m_{q} / a^{2}$ is allowed in $\langle\bar{\psi} \psi\rangle$ for staggered quarks, i.e. no term of the form $m_{q}^{2} / a$ can appear. In the ratio $R_{q}$ this term takes the form $C m_{q}^{2} / a^{2}$ where $C$ depends on the meson mass and decay constant. The HISQ formalism has


FIG. 4: $\quad R_{q}$, defined as the ratio of quark mass times condensate in the $\overline{M S}$ scheme at 2 GeV to the square of the meson mass times decay constant, as a function of the square of the inverse lattice spacing. Left to right and top to bottom shows strange quarks and light quarks with masses $m_{s} / 5, m_{s} / 10$ and the physical value. Squares use the unsubtracted condensate, pluses, the condensate after subtraction of the tree-level perturbative correction and crosses, the condensate after perturbative correction through one-loop. The value for $\alpha_{s}$ used to multiply the one-loop coefficient was $\alpha_{V}^{n_{f}=4}(2 / a)$. Dashed lines illustrate very simple linear fits to the unsubtracted results as described in the text.
very small discretisation errors, as is clear from the decay constant and meson mass results in [25, and so there is little additional $a$-dependence to confuse the analysis of the divergent pieces.

Because the power divergence is so dominant it is tempting to try to fit the unsubtracted results for $R_{s}$ to a very simple form: $A+B / a^{2}$. This is in fact possible (it is important to include the error in the inverse lattice spacing when doing this since this is larger than the error in $R_{q}$ ) and we obtain $1.02(3)+0.725(3) / a^{2}$ which is the dashed line in lefthand plot of Fig. 4. We also obtain $1.015(11)+0.229(5) / a^{2}$ for $R_{l}$ with $m_{l}=m_{s} / 5$ and $1.00(1)+0.130(6) / a^{2}$ for $R_{l}$ with $m_{l}=m_{s} / 10$, shown in the next two plots in Fig. 4. These fits are too naive to be useful, as we shall see below, because they miss out many important terms. Consequently the value and error of the intercept, $A$, is unreliable for extracting a nonperturbative result for $R_{q}$, especially in the $s$ quark case. However, the fits do illustrate that the ratio of
slopes is that expected for a term that behaves as $m_{q}^{2} / a^{2}$ (although the simple fit does not allow for the running of the lattice bare quark mass with scale). The ratio of slopes between that for $s$ and for $l$ with $m_{l}=m_{s} / 5$ is 3.2 which corresponds approximately to 5 (for the ratio of one power of the quark masses when the other power is cancelled by the square of the meson mass) divided by the ratio of the square of the decay constants from Table III

Figure 4 compares results for $R_{q}$ in which the tree-level piece of $\Delta_{P T}$ has been subtracted from the raw values of $m\langle\bar{\psi} \psi\rangle$ following Eq. 22 We take $\mu$ to be 2 GeV . These results are indicated by pluses. Now the slope in $a^{-2}$ is much smaller since the most of the divergence has been removed. This makes the results more sensitive to the form of the remaining pieces of the divergence and the simple linear fits that were made to the unsubtracted data are no longer possible.

The $\mathcal{O}\left(\alpha_{s}\right)$ perturbative contribution is very small for


FIG. 5: Finite volume effects in different quantities are illustrated by plotting the ratio of the quantity on lattices of spatial length, $L / a$, of 24 and 32 to that on lattices of spatial length 40. The lattices have the sea quark mass parameters of coarse set 5 . The quantities shown are the pion mass (red pluses), pion decay constant (green crosses) and unsubtracted light quark condensate (blue bursts). Pink squares give the result for the quantity $R_{l}$ defined in Eq. (23) [29]. Statistical errors (not shown) are approximately $0.1 \%$.

HISQ quarks and makes very little difference to the perturbative subtraction. The crosses show the results taking $\Delta_{P T}$ to be the full calculated perturbative subtraction through $\mathcal{O}\left(\alpha_{s}\right)$ given in Eq. 21. We have used $\alpha_{V}^{n_{f}=4}(2 / a)$ [30] for the $\alpha_{s}$ value multiplying the oneloop coefficient, but the coefficient itself is so small that variations in scale for $\alpha_{s}$ make no difference. The crosses are barely distinguishable from the pluses giving the treelevel subtracted numbers.

It is clear from Fig. 4 that there is still some divergence in $a^{-2}$ left in $R_{q}$ after subtraction of the perturbative contribution through one-loop. This is not surprising since we know that $\Delta_{P T}$ will have higher order terms in $\alpha_{s}$. The challenge now is to fit the one-loop subtracted $R_{q}$ allowing for these higher order terms and thereby obtain the physical, nonperturbative, results for the strange and light quark condensates. We will fit both $R_{s}$ and $R_{l}$ simultaneously and use the known mass dependence of the unknown higher order terms to constrain them. At the same time we will allow for higher-order non-divergent mass-dependent terms from perturbation theory as well as physical, non-perturbative, dependence on the quark mass. Possible dependence on positive powers of $a$, i.e. discretisation errors, must also be included.

## 2. Determining a physical result from fitting

We now describe the full fit to the results that we use to determine the final physical values for $\langle\bar{s} s\rangle\left(\equiv\left\langle\bar{\psi} \psi_{s}\right\rangle\right)$ and $\langle\bar{l}\rangle\rangle\left(\equiv\left\langle\bar{\psi} \psi_{l}\right\rangle\right)$ at the physical strange and light quark masses (where $m_{l}=\left(m_{u}+m_{d}\right) / 2$ ). We take the following
form for the ratio $R_{q}$ :

$$
\begin{equation*}
R_{q, 0}\left(a, a m_{q}\right)=R_{\mathrm{NP}, \mathrm{phys}}^{(q)}+\delta R_{P T}+\delta R_{a^{2}}+\delta R_{\chi}+\delta R_{\mathrm{vol}} \tag{25}
\end{equation*}
$$

$R_{q, 0}$ are the raw results obtained from Table $\Pi$ I $R_{\mathrm{NP}, \text { phys }}$ is the final physical result in the $\overline{M S}$ scheme at 2 GeV . The $\delta R$ terms represent fitted or known dependence on $a$ and $a m_{q}$. We use Bayesian techniques (31 to perform the fits so that we can add many higher order terms as part of each $\delta R$ with constrained coefficients. This makes sure that the final error on $R_{\mathrm{NP}, \text { phys }}$ is not underestimated by ignoring the existence of higher order corrections.
$\delta R_{P T}$ contains the known tree-level and one-loop perturbative results given in section IIIA. In addition we include unknown higher-order terms. For the $a^{-2}$ divergence these take the form:

$$
\begin{equation*}
\delta R_{P T, d i v}=a_{n} \frac{4 \alpha_{s}^{n}\left(a m_{q}\right)^{2}}{\left(a f_{\pi}\right)^{2}\left(a M_{\pi}\right)^{2}} \tag{26}
\end{equation*}
$$

with the analogous term for the strange quark case, with the same $a_{n}$. $a_{n}$ is a coefficient whose prior we take to be $0.0 \pm 4.0$ and we allow for $n=2,3$ and 4 . Note that a prior width of 4.0 is conservative given the size of the corresponding coefficient at tree-level and one-loop. For the non-divergent pieces we take:

$$
\begin{equation*}
\delta R_{P T, \text { non-div }}=c_{n} \frac{4 \alpha_{s}^{n}\left(a m_{q}\right)^{4}}{\left(a f_{\pi}\right)^{2}\left(a M_{\pi}\right)^{2}} \tag{27}
\end{equation*}
$$

again with the analogous term for the strange quark case, with the same coefficient $c_{n}$. We take $n=2,3$ and 4. $c_{n}$ in principle contains a sum of powers of $\log (a \mu)$ up to $\log ^{n+1}(a \mu)$. However, since $\log (a \mu)$ is small for $\mu=2 \mathrm{GeV}$ and our range of lattice spacings, these pieces are negligible and do not affect the fit and we simply take a prior on $c_{n}$ of $0.0(4.0)$. Again this is conservative given the results at tree-level and one-loop. For $\alpha_{s}$ we use $\alpha_{V}^{n_{f}=4}(2 / a)[30$ and discuss below the dependence of the results on changing $2 / a$ to a different scale. $\alpha_{V}^{n_{f}=4}(2 / a)$ takes values from 0.35 on the very coarse lattices to 0.26 on the fine ensembles.
$\delta R_{a^{2}}$ allows for discretisation errors. We take the form

$$
\begin{equation*}
\delta R_{a^{2}}=\sum_{i=1}^{2} d_{i}\left(\frac{\Lambda a}{\pi}\right)^{2 i} \tag{28}
\end{equation*}
$$

Only even powers of $a$ appear in discretisation errors for staggered quarks and we take their scale to be set by $\Lambda \approx$ 1 GeV . Since all tree level errors at $\mathcal{O}\left(a^{2}\right)$ are removed in the HISQ formalism we take the prior for $d_{1}$ to be $\mathcal{O}\left(\alpha_{s}\right)$ i.e. $0.0(0.3)$. Higher order $d_{i}$ are given the prior $0.0(1.0)$. We include $a^{2}$ and $a^{4}$ terms, but have checked that higher order terms have very little effect. In addition we include a mass-dependent discretisation error in the form $e(a m)^{2}$, giving $e$ a prior of $0.0(1.0)$. This allows for a number of effects, one of which could be mixing with a gluon condensate. This has negligible impact.
$\delta R_{\chi}$ includes the valence and sea quark mass dependence that allows us to extrapolate to physical light quark masses and interpolate between the strange quark masses that we have to the physical strange quark mass. The chiral corrections to the GMOR relation were analysed in [27] (see also [28]). The leading corrections are particularly simple because the chiral logarithms cancel to leave a correction proportional to $M_{\pi}^{2}$. We allow for both $M_{\pi}^{2}$ and $M_{\pi}^{4}$ terms in our light quark mass fits by defining a chiral expansion parameter

$$
\begin{equation*}
x_{l}=\frac{M_{\pi}^{2}}{2\left(\Lambda_{\chi}\right)^{2}} \tag{29}
\end{equation*}
$$

with $\Lambda_{\chi}=1.0 \mathrm{GeV}$, and taking

$$
\begin{equation*}
\delta R_{\chi, v a l}=\sum_{i=1}^{2} g_{i}^{(l)} x_{l}^{i} \tag{30}
\end{equation*}
$$

We fit the $m_{q}=m_{s} / 5, m_{s} / 10$ and $m_{l, p h y s}$ results with this form taking the prior on the $g_{i}$ coefficients to be $0.0(2.0)$. This allows for a linear term of approximately the size expected in [28]. Higher order terms than $x_{l}^{2}$ have no effect.

The chiral expansion of Eq. 30) combines with the $R_{\text {NP,phys }}$ parameter in Eq. 25 to define the physical nonperturbative light condensate with its mass dependence. Since the GMOR relation is exact as $m_{q} \rightarrow 0$ we enforce this by taking the prior on $R_{\mathrm{NP} \text {, phys }}^{(l)}$ to be $1.0000(5)$. Differences from 1 because of residual lattice finite volume effects up to $0.5 \%$ are allowed for as described in the paragraph above.

The data for $R_{s}$ is fit simultaneously with that for the light quarks, because they share parameters for the perturbative subtraction. However, we largely decouple the physical parameters because the strange quark is relatively far from the chiral limit and we would need a lot of parameters for a chiral expansion to connect light and strange quarks. Instead we allow a separate parameter for $R_{\mathrm{NP}, \text { phys }}^{(s)}$ with the broad prior of $1.0(5)$. We take the same form for the valence mass dependence as in Eq. (30) where now

$$
\begin{equation*}
x_{s}=\frac{\left(M_{\eta_{s}}^{2}-(0.6893(12))^{2}\right)}{2\left(\Lambda_{\chi}\right)^{2}} \tag{31}
\end{equation*}
$$

but this now simply allows for slight mistuning of the strange quark on some ensembles, and the fact that we have two values for the strange quark mass on sets 1 and 2. 0.6893 is the physical value for the $\eta_{s}$ mass determined in [25]. The priors on $g_{i}^{(s)}$ are the same as those on $g_{i}^{(l)}$. Finite volume effects are expected to be completely negligible for $R_{s}$ because they are negligible for the components of $R_{s}$.

The strange quark results in Fig. 4 show some very small sensitivity to the sea light quark masses if we compare results on sets 1 and 2 and sets 3 and 4 . We therefore
allow an additional linear dependence on the light quark mass in the sea in $\delta R_{\chi}$ of the form

$$
\begin{equation*}
\delta R_{\chi, \text { sea }}=\sum_{i=1}^{2} k_{i}\left(\frac{\delta m_{\text {sea }}}{10 m_{s, p h y s}}\right)^{i} \tag{32}
\end{equation*}
$$

where

$$
\begin{equation*}
\delta m_{\text {sea }}=\left(2 m_{l, \text { sea }}+m_{s, \text { sea }}\right)-\left(2 m_{l, p h y s}+m_{s, p h y s}\right) . \tag{33}
\end{equation*}
$$

We take $m_{l, p h y s}=m_{s} / 27.4$ 32 and $m_{s, p h y s}$ values determined from $M_{\eta_{s}}$ as in [25]. The prior for coefficient $k_{i}$ is taken as $0.0(1.0)$ which is conservative given the small effects observed in the results. We take $\delta R_{\chi, \text { sea }}$ to be common to both $R_{s}$ and $R_{q}$ for the light quarks. We note here also that the absence of chiral loop effects at this order means that staggered quark taste-changing effects are also absent. They can be handled, if necessary, with a sea-quark mass dependent $a^{2}$ term [25]. Including such a term here makes no difference to the physical result.
$\delta R_{\mathrm{vol}}$ allows for remaining finite volume effects. These are small, as demonstrated in Fig. 5. They do produce a small systematic effect, however, because the lattice size in units of the pion mass, $M_{\pi} L$, is somewhat smaller on the lattices with smallest $m_{u / d}$. We take:

$$
\begin{equation*}
\delta R_{\mathrm{vol}}=v e^{-M L} \tag{34}
\end{equation*}
$$

where $M$ is the pseudoscalar meson mass made of that quark ( $M_{\pi}$ for $R_{l}$ and $M_{\eta_{s}}$ for $R_{s}$ ) and $L$ is the linear extent of the lattice from Table I. Coefficient $v$ is taken to have prior $0.0(0.2)$, consistent with Fig. 5 .

Fitting $R_{s}$ and $R_{q}, m_{q}=m_{s} / 5, m_{s} / 10$ and $m_{l, p h y s}$, results simultaneously to the form in Eq. (25) readily produces good fits with $\chi^{2} /$ dof $\approx 0.8$ for 18 degrees of freedom. The final fitted result for $R_{u / d}$ and $R_{s}$ (evaluated from $R_{\mathrm{NP}, \mathrm{phys}}^{(q)}$ and $\delta R_{\chi}$ taken at the appropriate physical masses) is robust to the addition of higher order terms in the various corrections.

We take our final results from using $2 / a$ for the scale of $\alpha_{s}$. The results do not change significantly as this is varied (although the fitted coefficients $a_{n}$ do change). Our fits return a substantial value for the coefficient of the power divergent term at $\mathcal{O}\left(\alpha_{s}^{2}\right), a_{2}$, of around 2.0, for $d / a=2 / a$. This is substantially larger than that seen at one-loop but not a particularly large value for a perturbative coefficient in general. It would simply imply that the small coefficient at one-loop for the HISQ action is not repeated at higher orders. We also find that the chiral correction to the GMOR for light quarks is substantial and negative $\left(g_{1}^{(l)}=-1.7(6)\right)$. This will be discussed further below.

The fit results are shown in Fig. 6. The data points (crosses) correspond to the lattice QCD results after subtraction of the perturbative contribution through $\mathcal{O}\left(\alpha_{s}\right)$ (as in Fig. 4). The filled bands show the fitted curves when the full fitted perturbative contribution $\left(\delta R_{P T}\right)$ is

TABLE IV: Error budget for the quantities $R_{s, p h y s}, R_{l, p h y s}$ and their ratio defined in the text. Errors are given as percentages of the final physical result.

|  | $R_{s, p h y s}$ | $R_{l, p h y s}$ | $\frac{R_{s, p h y s}}{R_{l, p h y s}}$ |
| :--- | :--- | :--- | :--- |
| statistics | 6.1 | 0.2 | 5.1 |
| lattice spacing | 10.0 | 0.3 | 9.7 |
| finite volume | 1.5 | 0.03 | 1.5 |
| $\alpha_{s}$ value | 1.7 | 0.06 | 1.7 |
| fitting power divergence | 7.5 | 0.3 | 7.2 |
| other perturbative subtraction | 1.3 | 0.07 | 1.3 |
| خal extrap./interp. $\left(m_{s}\right)$ | 3.0 | 0.1 | 2.9 |
| خal extrap./interp. $\left(m_{l}\right)$ | 4.5 | 0.2 | 4.3 |
| $a \rightarrow 0$ extrap. | 1.9 | 0.05 | 1.9 |
| sea mass effects | 0.5 | 0.01 | 0.5 |
| Total | 15 | 0.5 | 14.5 |

subtracted and masses and decay constants are set to the physical values corresponding to the $s$ quark and the light quark (for this we use $M_{\pi}=M_{\pi^{0}}$ ). These bands include the full error from the fit.

Our final physical results for $R_{q}$ are the key results from this paper.

$$
\begin{align*}
R_{l, p h y s} & =-\frac{4 m_{l}\left\langle\bar{\psi} \psi_{l}\right\rangle_{\overline{M S}}(2 \mathrm{GeV})}{\left(f_{\pi}^{2} M_{\pi}^{2}\right)} \\
R_{s, p h y s} & =-\frac{4 m_{s}\left\langle\bar{\psi} \psi_{s}\right\rangle_{\overline{M S}}(2 \mathrm{GeV})}{\left(f_{\eta_{s}}^{2} M_{\eta_{s}}^{2}\right)} \tag{35}
\end{align*}
$$

We find:

$$
\begin{align*}
R_{s, p h y s} & =0.574(86) \\
R_{l, p h y s} & =0.985(5) \\
\frac{R_{s, p h y s}}{R_{l, p h y s}} & =0.583(84) \tag{36}
\end{align*}
$$

The complete error budgets for $R_{s, p h y s}, R_{l, p h y s}$ and their ratio are given in Table IV. The substantial $15 \%$ error that we have in $R_{s, p h y s}$ reflects the difficulty of extracting a physical result from a power divergent quantity. For $R_{l}$ the error is 17 times better largely because the slope of the divergent piece is 15 times smaller. Errors in $R_{s, p h y s}$ are dominated by errors from the lattice spacing and from fitting the remaining power divergent subtraction terms. There are also substantial errors from statistics and from tuning to the light and strange physical mass points. This is done by tuning the appropriate meson masses through the term $\delta R_{\chi, v a l}$ in Eq. 30. This term depends on the lattice spacing through the definition of $x_{l}$ (Eq. 29) and $x_{s}$ (Eq. 31), because the meson masses appear in GeV units in these terms. The uncertainties in these terms then becomes correlated with the fit to the power divergence, increasing the uncertainty. For $R_{l}$ the power divergence is much less of an issue, but these same terms dominate the final error there as well.


FIG. 6: Results from fitting the ratio $R$ for three different quark masses as described in the text. The crosses show the lattice QCD results after subtracting the perturbative values through $\mathcal{O}\left(\alpha_{s}\right)$. Black is for $s$ quarks, blue for quarks with mass $m_{s} / 5$, red for quarks with mass $m_{s} / 10$ and green for quarks at the physical light quark mass. The dashed lines simply join the points of matching color for clarity. The filled bands show the physical curves for strange (black) and light (green) quarks, once the full subtraction of the fitted perturbative contribution is made and masses are set to their physical values. The bands include the full error from the fit.

The results for $R_{l}$ and $R_{s}$ can be converted to values of the condensate using the lattice result for $f_{\eta_{s}}=0.1819(5)$ GeV and $M_{\eta_{s}}=0.6893(12) \mathrm{GeV}$ [25], and experimental values for $f_{\pi}(0.1304(2) \mathrm{GeV})$ and $M_{\pi}(0.13498 \mathrm{GeV})$. We obtain:

$$
\begin{align*}
m_{s}\langle\bar{\psi} \psi\rangle_{s}^{\overline{M S}}(2 \mathrm{GeV}) & =-2.26(34) \times 10^{-3} \mathrm{GeV}^{4} \\
m_{l}\langle\bar{\psi} \psi\rangle_{l}^{\overline{M S}}(2 \mathrm{GeV}) & =-7.63(4) \times 10^{-5} \mathrm{GeV}^{4} \tag{37}
\end{align*}
$$

The ratio of the two values above is slightly more accurate than a naive combination, giving 29.6(4.3).

Using the precise determinations for light quark masses now available from lattice QCD we can finally obtain condensate values. We take $m_{s}^{\overline{M S}}(2 \mathrm{GeV})=92.2(1.3)$ MeV [30, 33] and $m_{s} / m_{l}=27.41(23)$ [32, 34]. These give:

$$
\begin{align*}
\langle\bar{s} s\rangle^{\overline{M S}}(2 \mathrm{GeV}) & =-0.0245(37)(3) \mathrm{GeV}^{3} \\
& =-(290(15) \mathrm{MeV})^{3} \\
\langle\bar{l} l\rangle^{\overline{M S}}(2 \mathrm{GeV}) & =-0.0227(1)(4) \mathrm{GeV}^{3} \\
& =-(283(2) \mathrm{MeV})^{3}, \tag{38}
\end{align*}
$$

where the second error for each condensate in $\mathrm{GeV}^{3}$ comes from the error in the quark masses.

For the ratio of strange to light condensate we have:

$$
\begin{equation*}
\frac{\langle\bar{s} s\rangle^{\overline{M S}}(2 \mathrm{GeV})}{\langle\bar{l} l\rangle^{\overline{M S}}(2 \mathrm{GeV})}=1.08(16)(1) \tag{39}
\end{equation*}
$$

where the first error comes from $R_{s} / R_{l}$ and has the error budget given in Table $\overline{I V}$ and the second error comes from the strange to light quark mass ratio.

## 3. Approach of $R$ to the chiral limit

The relationship of the light quark condensate to the chiral condensate is also important. $R_{q}$ is defined to have the value 1 from the GMOR relation in the chiral limit but the results of Eq. 36 indicate that it approaches this limit from below as the light quark mass is reduced. Supporting evidence for this is found by studying the quantity $R_{\delta}$ derived from the combination of condensates used by the HOTQCD collaboration in their study of finite temperature QCD [35]. We define $R_{\delta}$ by:

$$
\begin{equation*}
R_{\delta}=\frac{4 m_{l}}{f_{\pi}^{2} M_{\pi}^{2}} \frac{\left\langle\bar{\psi} \psi_{l}\right\rangle-\frac{m_{l}}{m_{s}}\left\langle\bar{\psi} \psi_{s}\right\rangle}{1-\frac{m_{l}}{m_{s}}} \tag{40}
\end{equation*}
$$

The quadratic divergence with lattice spacing cancels between the two condensates because it is linear in the quark mass to all orders in perturbation theory. The non-divergent perturbative contributions proportional to the cube of the quark mass are completely negligible here, from the perturbative analysis in section III A, and so we do not need to include them in making $R_{\delta}$ a physical quantity. $R_{\delta}$ can then simply be calculated from the raw data in Table III


FIG. 7: $R_{\delta}$ as a function of $m_{l} / m_{s}$ at three values of the lattice spacing. Points show the raw lattice results: the crosses are from very coarse lattices (sets 1 and 2 with two values of $m_{s}$ on each and set 3 ), open circles from coarse lattices (sets 4,5 and 6 ) and open triangles from fine sets 7 and 8 . The shaded band gives the results of a simple fit incorporating discretisation and finite volume effects as described in the text.

A plot of $R_{\delta}$ against $m_{l} / m_{s}$ is shown in Fig. 7. In the $m_{l} \rightarrow 0$ limit on an infinite volume $R_{\delta} \rightarrow 1$ as $R_{l}$ does. $R_{\delta}$ can be determined more precisely than $R_{l}$, however, because of the nonperturbative cancellation of the power divergence and it clearly approaches 1 from below. $R_{\delta}$ differs from $R_{l}$ by a term which is proportional to $m_{l} / m_{s}$ and to the difference between $\langle\bar{s} s\rangle$ and $\langle\bar{l} l\rangle$. Both the dependence of $R_{l}$ on $m_{l}$ and the difference between $R_{\delta}$ and $R_{l}$ then contribute to the slope with $m_{l}$ seen in Fig. 7 . We cannot separate them and therefore unambiguously identify the slope of $R_{l}$ with $m_{l}$. We can however use this for a consistency check.

We fit $R_{\delta}$ to the simple form:

$$
\begin{align*}
R_{\delta} & =1.000(1)+c_{1}\left(1+c_{2} a^{2}+c_{3} a^{4}\right) \frac{m_{l}}{m_{s}} \\
& +c_{4}\left(\frac{m_{l}}{m_{s}}\right)^{2}+c_{5} e^{-m_{\pi} L} \tag{41}
\end{align*}
$$

This allows for linear and quadratic terms in $m_{l}$ with discretisation errors. We take priors on $c_{1}, c_{3}$ and $c_{4}$ to be $0.0(1.0)$ and prior on $c_{2}$ to be $0.0(0.3)$ consistent with $\alpha_{s} a^{2}$ behaviours. The final term allows for finite volume effects dependent on the combination $m_{\pi} L$. As for our fit to $R_{l}$, we take the prior on $c_{5}$ to be $0.0(0.2)$ for consistency with Fig. 5

The fit gives $\chi^{2}$ /dof of 0.75 for 10 degrees of freedom and a physical slope, $c_{1}$, of $-0.51(4)$. This value is consistent with the difference between $R_{l}$ and 1 in Eq. 36 , and indeed with the difference between $R_{s}$ and 1. This consistency between the results from $R_{\delta}$ and $R_{l}$ indicates that the difference between $\langle\bar{s} s\rangle$ and $\langle\bar{l} l\rangle$ (which would upset this consistency) cannot be large. This is indeed what we also find in Eq. 39 .

## 4. The chiral susceptibility

A further quantity that is of particular interest in studies of QCD at finite temperature is the chiral susceptibility for a quark of flavor $f$ :

$$
\begin{equation*}
\chi_{f}=\frac{\partial}{\partial m_{f}}\left(-\left\langle\bar{\psi} \psi_{f}\right\rangle\right) . \tag{42}
\end{equation*}
$$

We give results here for the chiral susceptibility for zero temperature QCD to fill out the physical picture of the condensate. From differentiation of the path integral for the condensate it is clear that the chiral susceptibility is given by the flavor-singlet scalar correlator. It is convenient to split this into two contributions which we call $\chi_{q}$ and $\chi_{g}{ }^{1} . \chi_{q}$ comes from two scalar operators connected by quark lines, which is the flavor-nonsinglet scalar meson correlator. $\chi_{g}$ comes from two scalar operators con-

[^306]TABLE V: Contributions to the chiral susceptibility, defined in Eq. (44) for very coarse set 1 and coarse set 4 for light ( $m_{l}=m_{s} / 5$ ) and strange quark masses.

| Set | $m a$ | $a^{2} \chi_{q}$ | $a^{2} \chi_{g}$ |
| :--- | :--- | :--- | :--- |
| 1 | 0.013 | $0.54296(36)$ | $0.045(14)$ |
|  | 0.0688 | $0.45359(6)$ | $0.021(7)$ |
| 3 | 0.01044 | $0.50850(18)$ | $0.032(10)$ |
|  | 0.0522 | $0.46231(3)$ | $0.014(4)$ |

nected only by gluons, in which the disconnected contribution is cancelled.

$$
\begin{align*}
\chi & =\chi_{q}+\chi_{g}  \tag{43}\\
\chi_{q} & =\frac{1}{N_{t}} \sum_{n} \operatorname{Tr}\left[M_{0 n}^{-1} M_{n 0}^{-1}\right] \\
\chi_{g} & =-\frac{1}{N_{t}^{2} V}\left(\left\langle\left(\operatorname{Tr} M^{-1}\right)^{2}\right\rangle-\left\langle\operatorname{Tr} M^{-1}\right\rangle^{2}\right)
\end{align*}
$$

The factors of number of tastes, $N_{t}$, above are specific to naive/staggered quarks.


FIG. 8: Results for the quark-line connected scalar correlator on set 1: $s$ quarks (blue crosses) and light quarks with $m_{l}=$ $m_{s} / 5$ (red bursts). The sum over time of this correlator is $\chi_{q}$. Negative values of the correlator are not plotted on this log scale.
$\chi_{q}$ is readily calculated by generating quark propagators with the same random wall source of noise as that used for the $\pi$ and $\eta_{s}$ mesons, but patterned with phases that are -1 on all odd sites on an even-odd partitioning of the lattice. We then combine one of these propagators with the matching one used in the $\pi / \eta_{s}$ meson, again multiplying the odd sink sites with a phase of -1 . Summing over spatial sites at each time slice gives the flavor-nonsinglet scalar correlator. Examples are shown


FIG. 9: Results for the gluon-connected contribution to the scalar correlator on set 1 for $s$ quarks (blue crosses) and light quarks with $m_{l}=m_{s} / 5$ (red bursts). The sum over time of this correlator is $\chi_{g}$.
in Fig. 8. Summing this correlator over time slices gives $\chi_{q}$. Results for $\chi_{q}$ for light and strange quarks on sets 1 and 4 are given in Table V
$\chi_{g}$ can be estimated from our existing results for the light and strange condensates. Because we have 16 time sources for our propagators we can determine the correlation between $\operatorname{Tr} M^{-1}$ operator that are $n$ time slices apart where $n$ is a multiple of 3 for set 1 and a multiple of 4 for set 4 . This gives a correlation function, for example that shown in Figure $9 . \chi_{g}$ is then the sum over time slices of this correlation function. We can estimate $\chi_{g}$ in several ways. Our central result comes from estimating an effective mass from the early time slices that dominate $\chi_{g}$ and where we have a strong signal. We can then reconstruct an estimated correlation function and sum over it. We can also simply sum over the correlator for the time slices that we have and multiply by 3 or 4 as appropriate. From this range of methods we estimate the error in $\chi_{g}$ as $30 \%$. Values are given in Table V. $\chi_{g}$ is much smaller than $\chi_{q}$.

The quantities that are almost Renormlisation-Group invariant, that we can compare, are $m_{f}^{2} \chi_{f}$ and $m_{f}\left(-\left\langle\bar{\psi} \psi_{f}\right\rangle\right.$. This is done in Figure 10 . Both of these quantities contain the same power divergence (proportional to $m_{f}^{2} a^{-2}$ ) in the lattice spacing. In the susceptibility this divergence largely comes from $\chi_{q}$. The nondivergent perturbative contributions to the two quantities will be different but, as we have seen, they are very small and we ignore them here.

We find that the difference between $m_{f}^{2} \chi_{f}$ and $-m_{f}\left\langle\bar{\psi} \psi_{f}\right\rangle$, also plotted in Figure 10, does not depend on the lattice spacing within errors. We simply average over the results at the two values of the lattice spacing


FIG. 10: Results for $m_{f}^{2} \chi_{f}$ (open circles) compared to $m_{f}\left\langle\bar{\psi} \psi_{f}\right\rangle$ (open triangles) as a function of the square of the inverse lattice spacing, for $s$ quarks (top) and light quarks with $m_{l}=m_{s} / 5$ (lower plot). Results are for sets 1 and 4 . Bursts show the difference of these two quantities.
to obtain physical results for

$$
\begin{equation*}
m_{f}\left(1-m_{f} \frac{\partial}{\partial m_{f}}\right)\left\langle-\bar{\psi} \psi_{f}\right\rangle \tag{44}
\end{equation*}
$$

The values are: $2.18(7) \times 10^{-3} \mathrm{GeV}^{4}$ for $s$ quarks and $3.93(9) \times 10^{-4} \mathrm{GeV}^{4}$ for light quarks with $m_{l}=m_{s} / 5$. Comparison of these numbers with the physical results for $m_{f}\left\langle\bar{\psi} \psi_{f}\right\rangle$ given in Eq. 37$\rangle$ allows us to determine the value and sign of $m_{f}^{2} \chi_{f}$. For $s$ quarks the comparison is straightforward and we find:

$$
\begin{equation*}
m_{s}^{2} \chi_{s}=0.08(35) \times 10^{-3} \mathrm{GeV}^{4} \tag{45}
\end{equation*}
$$

consistent with zero.
To obtain a value for $m_{l}^{2} \chi_{l}$ at $m_{l}=m_{s} / 5$ we need a result for $m_{l}\left\langle\bar{\psi} \psi_{l}\right\rangle$ at this mass. Our fit in Sec. III B 2 gives a result for $R_{l=s / 5}$ of $0.915(26)$. At this value of $m_{l}$ we have $M_{\pi}=315 \mathrm{MeV}$ and can estimate $f_{\pi}=145 \mathrm{MeV}$ from our results in Table II. Then $m_{l=s / 5}\left\langle\bar{\psi} \psi_{l=s / 5}\right\rangle=$ $4.78(20) \times 10^{-4} \mathrm{GeV}^{4}$. In the error we have included an
interpolation error for each of the mass and decay constant of $1 \%$. Then, subtracting the result for the difference of Eq. 44 at $m_{l}=m_{s} / 5$ given above, we have

$$
\begin{equation*}
m_{l=s / 5}^{2} \chi_{l=s / 5}=0.85(22) \times 10^{-4} \mathrm{GeV}^{4} \tag{46}
\end{equation*}
$$

which is a small positive slope.
Our results are then consistent with a slope in $\left\langle\bar{\psi} \psi_{f}\right\rangle$ with $m_{f}$ that is positive at $m_{s} / 5$ but may decrease or even become negative by $m_{s}$. If the slope at $m_{s} / 5$ remained constant for larger $m_{f}$ it would give a total change in $\left\langle\bar{\psi} \psi_{f}\right\rangle$ of $3 \times 10^{-3}$ between $m_{s} / 5$ and $m_{s}$ which is not inconsistent with the change of $1.8(3.8) \times 10^{-3}$ that we find in Eq. 38 .

## IV. DISCUSSION

We have determined a physical value for the strange quark condensate from lattice QCD for the first time. This required both nonperturbative lattice QCD results and a perturbative determination of the power divergent contribution through $\mathcal{O}\left(\alpha_{s}\right)$. The calculation relies on the good chiral properties of staggered quarks to control the form of the power divergence and the numerical speed and small discretisation of the Highly Improved Staggered quark formalism allow very precise results to be obtained at several values of the lattice with light $u / d$ sea quark masses. We proceed by tracking deviations from the GMOR relation, making extensive use of our previous work determining the physical properties of the $\eta_{s}$ meson, to obtain the strange quark condensate. Our best result comes from gluon field configurations that include $u, d, s$ and $c$ quarks in the sea. The condensate is given in the $\overline{M S}$ scheme at a scale of 2 GeV . The evolution equation required to run $m\langle\bar{\psi} \psi\rangle$ to other scales, since it is not RG-invariant, is given in Appendix B. We obtain a very consistent result for the strange quark condensate from independent calculations that include $2+1$ favors of sea quarks, as discussed in Appendix D.

Our value is $-(290(15) \mathrm{MeV})^{3}$ giving a ratio of strange to light condensates of $1.08(16)$. Earlier results come from sum rules of various kinds. These show significant variation and often have no estimate of the error associated with the value. Narison [36] gives a compilation with a final value for the ratio of strange to light condensates in the $\overline{M S}$ scheme at a scale of 2 GeV of $0.75(12)$. A value of $0.74(3)$ is quoted from baryon mass splittings in [11. Finite energy sum rules in the kaon sector give a ratio $0.6(1)$ in [37. More recently Maltman 12 ] uses sum rules for the ratio of decay constants $f_{B_{s}} / f_{B}$ along with the 2007 lattice QCD average for this ratio of $1.21(4)$ [38, 39 to obtain $\langle s \bar{s}\rangle /\langle l \bar{l}\rangle_{\overline{M S}}(2 \mathrm{GeV})=1.2(3)$. This updates an earlier result of $0.8(3)$ from Jamin [28] which used a quenched lattice QCD result for $f_{B_{s}} / f_{B}$ of $1.16(4)$. The current lattice QCD world average for $f_{B_{s}} / f_{B}$ is 1.20(2) 40.


FIG. 11: A comparison of results for the ratio of strange to light condensates in the $\overline{M S}$ scheme at 2 GeV .

Fig. 11 compares our result for the strange to light condensate ratio with the results from sum rules discussed above. Our central value lies between the sum rules results, being in agreement with the larger value of [12] but only in marginal agreement with the lower values of 37]. A value below 0.6 is ruled out by our results at the $3 \sigma$ level. Our value is more accurate than the result derived from $f_{B_{s}} / f_{B}$ and has the advantage over all the sum rules results that it is a direct determination from QCD and has a full error budget (Table IV).

We obtain a very accurate value for the light quark condensate, giving $-(283(2) \mathrm{MeV})^{3}$. We can distinguish the ratio $R_{l}$ at the physical light quark mass from that of 1 in the chiral limit using our results in Eq.( 36 ). Defining $\delta_{\pi}$ from [28]

$$
\begin{equation*}
R_{l}=1-\delta_{\pi} \tag{47}
\end{equation*}
$$

we obtain a value $\delta_{\pi}=0.015(5)$. This is somewhat lower than the value of 0.047 (17) estimated in [28], although in agreement within $2 \sigma$. It is not in agreement with the somewhat larger number of 0.06(1) obtained in 41]. Our result implies a value for the combination $\left(2 L_{8}^{r}-H_{2}^{r}\right)$ of low energy constants from the chiral Lagrangian that is a factor of three lower than that used in [28]. The value is $3 \sigma$ larger than zero, however.

Note that we do not expect the value of the light quark condensate to agree with that of the chiral (zero quark mass) condensate, $\Sigma$. The relationship between them is:

$$
\begin{equation*}
\Sigma(2 \mathrm{GeV})=\frac{-\langle\bar{l} l\rangle(2 \mathrm{GeV})}{R_{l, p h y s}} \frac{f^{2}}{f_{\pi}^{2}} \frac{\left(M^{2} / m\right)_{m=0}}{M_{\pi}^{2} / m_{l, p h y s}} \tag{48}
\end{equation*}
$$

Here $f$ is the decay constant in the zero quark mass limit and $M^{2} / m$ is the ratio of the square of the pion mass to the light quark mass in the same limit. $f_{\pi} / f$ can be
determined from chiral extrapolation of lattice QCD results. For example, a recent accurate calculation [3] gives $f_{\pi} / f=1.0627(28)$ including $2+1$ flavors of sea quarks. A preliminary analysis based on the results given here for $2+1+1$ sea flavors in Table II gives 1.056(1), in acceptable agreement. From the figures in [3] we estimate $\left(M^{2} / m\right)_{m=0} /\left(M_{\pi}^{2} / m_{l, p h y s}\right)$ as 1.02. Combining these factors, along with $R_{l}$, into Eq. 48 makes clear that we expect a $3 \%$ difference between the magnitudes of $\Sigma^{1 / 3}$ and $(\langle\bar{l} l\rangle)^{1 / 3}$, dominated by the effect of $f_{\pi} / f$ (so that $\Sigma$ is smaller). This is entirely consistent, assuming no difference between $2+1$ and $2+1+1$ flavors of sea quarks, with the fact that we obtain $\langle\bar{l} l\rangle(2 \mathrm{GeV})=-(283(2) \mathrm{MeV})^{3}$ and [3] obtain $\Sigma(2 \mathrm{GeV})=(272(2) \mathrm{MeV})^{3}$ from a chiral analysis.

Other methods for determining $\Sigma$ are not as accurate, but in reasonable agreement. We quote here two recent examples. JLQCD/TWQCD give a result of $(234(17) \mathrm{MeV})^{3}$ [42 from the eigenvalue spectrum of overlap quarks with $u, d$ and $s$ quarks in the sea. The ETM collaboration give $(299(38) \mathrm{MeV})^{3}$ [43] from fits to the Landau gauge quark propagator with $u$ and $d$ quarks in the sea. Additional lattice results for $\Sigma$ are collected in 44.

Our analysis has implications for other calculations. For example:

- Finite temperature determinations of the chiral phase transition in QCD use an order parameter based on the light quark condensate. A nonperturbative subtraction is made with the aim of removing the power divergent pieces proportional to $m a$ and with the assumption that the higher order $\left((m a)^{3}\right)$ terms are negligible. For example the HOTQCD collaboration uses an order parameter [35] for visualising the transition (fits to find the transition temperature also include other results) which is the ratio between non-zero and zero temperature of

$$
\begin{equation*}
\langle\bar{\psi} \psi\rangle_{l}-\frac{m_{l}}{m_{s}}\langle\bar{\psi} \psi\rangle_{s} . \tag{49}
\end{equation*}
$$

This quantity becomes

$$
\begin{equation*}
\langle\bar{\psi} \psi\rangle_{l, N P}-\frac{m_{l}}{m_{s}}\langle\bar{\psi} \psi\rangle_{s, N P} \tag{50}
\end{equation*}
$$

if we assume only the presence of a power divergence linear in ma. Our analysis shows that this is a good assumption. For example, the difference between subtracting only terms linear in $m a$ at tree level and including terms cubic in $m a$ is $0.2 \%$ for the strange condensate on the coarsest HOTQCD lattices (i.e. those with largest $m_{s} a$ values). An alternative might be to calculate $(1-m \partial / \partial m)\langle\bar{\psi} \psi\rangle$ as discussed in Sec. IIIB4. The quark-line connected piece of this can be calculated directly by combining the expression for $\chi_{q}$ in Eq. 44 and the expression for $\langle\bar{\psi} \psi\rangle$ in Eq. 10 . The combination
becomes [26]:

$$
\begin{equation*}
\left(1-\frac{\partial}{\partial m}\right)_{\text {conn }}\langle-\bar{\psi} \psi\rangle=2 m \sum_{n \text { even }} \operatorname{Tr}\left|M_{0 n}^{-1}\right|^{2} \tag{51}
\end{equation*}
$$

This can clearly be generalised to a sum over even source sites, implemented with a partial random wall. When combined with the quark-line disconnected piece $\chi_{g}$ this gives a physical quantity without power divergent pieces which is close to the value of the condensate itself.

- The comparison of heavy-light current-current correlators to continuum QCD perturbation theory can be used to normalise heavy-light currents in lattice QCD. The light quark condensate appears in this comparison and the results given here will enable us to improve the analysis in 8. This is underway.
- Some recent papers 45 have speculated that the quark condensate may only be non-zero inside hadrons. A much smaller value outside hadrons would significantly ameliorate the fine tuning problem associated with the cosmological constant. This suggestion appears to be in conflict with direct calculations of quark condensates as vacuum expectation values described here.


## V. CONCLUSIONS

We give the first direct determination of the strange quark condensate from lattice QCD , having demonstrated how to extract a well-defined physical value from lattice results that contain a power divergence as the lattice spacing goes to zero. Our results include a calculation through $\mathcal{O}\left(\alpha_{s}\right)$ in lattice QCD perturbation theory of the perturbative contribution to the condensate, part of which is the power divergence. The calculation relies on the good chiral properties of staggered quarks to control the form of the power divergence and the numerical speed and small discretisation of the Highly Improved Staggered quark formalism to obtain precise results at multiple lattice spacings and light quark masses. Our results include values at physical light quark masses.

We obtain a value for the strange quark condensate in the $\overline{M S}$ scheme at 2 GeV of $-(290(15) \mathrm{MeV})^{3}$. We give a full error budget for this result in Table IV, the main sources of error being those associated with fitting and subtracting the remaining power divergence. The result includes $u, d, s$ and $c$ quarks in the sea but we get good agreement with this value from independent calculations that include $u, d$ and $s$ sea quarks only.

The value we obtain for the corresponding light quark condensate (where $\left.m_{l}=\left(m_{u}+m_{d}\right) / 2\right)$ is $-(283(2) \mathrm{MeV})^{3}$. Note that is significantly different from the value for the condensate in the chiral limit. The ratio of our light quark condensate to a recent lattice QCD
value for the chiral condensate from [3] is $1.13(3)$, consistent with the behaviour of meson masses and decay constants approaching the chiral limit.

We have shown that the ratio of four times the quark mass times condensate divided by the square of the meson mass times decay constant approaches the GMOR value (of 1) from below as $m_{l} \rightarrow 0$. At the physical light quark mass the value is $1.5 \%$ below 1 , and at the strange mass it is $57 \%$ of 1 .

Our result for the ratio of the strange condensate to the light quark condensate is $1.08(16)$. This sits in the middle of the spread of results from QCD sum rules but provides significant additional information because it is a direct determination with a full error budget. The result will have impact on a number of other calculations both in the continuum and in lattice QCD. Some of the numerical techniques used here will be useful for determinations of, for example, the strangeness content of the pion or nucleon.

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## Appendix A: Condensates from correlators

Eq. (11) relates the zero-momentum pseudoscalar propagator to the scalar quark-condensate and is a wellknown relationship [26]. The relationship is true (for the HISQ formalism) even on a single gluon configuration. Here, for completeness, we give a simple derivation, using the equivalent naive quark formalism.

The contribution to the propagator from a single gluon configuration is given by

$$
\begin{equation*}
G_{\mathrm{ps}} \equiv \sum_{x} \operatorname{Tr}\left[\gamma_{5}\left(\frac{1}{D \cdot \gamma+m}\right)_{0 x} \gamma_{5}\left(\frac{1}{D \cdot \gamma+m}\right)_{x 0}\right] \tag{A1}
\end{equation*}
$$

where $D$ is the gauge-covariant derivative, and the trace is over spin and color indices. The contribution to the scalar quark-condensate is given by

$$
\begin{equation*}
S \equiv-\operatorname{Tr}\left(\frac{1}{D \cdot \gamma+m}\right)_{00} \tag{A2}
\end{equation*}
$$

To extract the relationship, we multiply by the unit ma-
trix under the trace in the condensate:

$$
\begin{align*}
S= & -\sum_{x y} \operatorname{Tr}\left[(-D \cdot \gamma+m)_{0 x}\left(\frac{1}{-D \cdot \gamma+m}\right)_{x y} \times\right. \\
& \left.\left(\frac{1}{D \cdot \gamma+m}\right)_{y 0}\right] \\
= & -\sum_{x} \operatorname{Tr}\left[(-D \cdot \gamma+m)_{0 x}\left(\frac{1}{-(D \cdot \gamma)^{2}+m^{2}}\right)_{x 0}\right] \tag{A3}
\end{align*}
$$

Only the $m$ term in the numerator of the last expression survives the spinor trace since the other term results in traces of odd numbers of $\gamma$ matrices (which vanish). Consequently

$$
\begin{align*}
S & =-m \operatorname{Tr}\left(\frac{1}{-(D \cdot \gamma)^{2}+m^{2}}\right)_{00} \\
& =-m \sum_{x} \operatorname{Tr}\left[\left(\frac{1}{-D \cdot \gamma+m}\right)_{0 x}\left(\frac{1}{D \cdot \gamma+m}\right)_{x 0}\right] \\
& =-m \sum_{x} \operatorname{Tr}\left[\gamma_{5}\left(\frac{1}{D \cdot \gamma+m}\right)_{0 x} \gamma_{5} \times\right. \\
& =-m G_{\mathrm{ps}} \\
& \left.\left(\frac{1}{D \cdot \gamma+m}\right)_{x 0}\right] \tag{A4}
\end{align*}
$$

which is Eq. 11). Since this relationship is true configuration-by-configuration, it must be true of the ensemble averages as well.

Note that Eq. A4 leads immediately to the GMOR relation (Eq. (1)). To see this rewrite the pseudoscalar propagator in terms of its mesonic intermediate states. Only the pion contribution survives the $m \rightarrow 0$ limit, since the effective decay constants for excited states all vanish in that limit (by the Ward identity). The pion contribution has an amplitude $a=f_{\pi}^{2} m_{\pi}^{3} /(4 m)$ multiplied by an exponential decay in time, whose integral gives $1 / m_{\pi}$.

The analysis of the propagator above only works for quark actions that have a $\gamma_{\mu}$ piece and a scalar piece (and nothing else), and where those two pieces commute with each other. The commuting is essential if you want

$$
\begin{equation*}
(-D \cdot \gamma+m)(D \cdot \gamma+m)=-(D \cdot \gamma)^{2}+m^{2} \tag{A5}
\end{equation*}
$$

with only terms having an even number of $\gamma_{\mu} \mathrm{s}$ on the right hand side. So this proof does not work for Wilson's lattice discretization of the quark action or similar formulations. On the other hand, it is true of staggered-quark formalisms such as HISQ.

Eq.(11) also follows directly from the (integrated) axial Ward identity:

$$
\begin{array}{r}
\sum_{x}\left\langle\left(m_{a}+m_{b}\right) J_{a b}^{5}(x)\left(m_{a}+m_{b}\right) J_{a b}^{5 \dagger}(0)\right\rangle= \\
-\left\langle\left(m_{a}+m_{b}\right)\left(\overline{\psi_{a}} \psi_{a}+\overline{\psi_{b}} \psi_{b}\right)\right\rangle \tag{A6}
\end{array}
$$

with $J_{a b}^{5} \equiv \overline{\psi_{a}}(x) \gamma_{5} \psi_{b}(x)$. This is exact on the lattice for lattice actions with sufficient chiral symmetry and again shows that is an identity, true configuration by configuration and for any $m_{a}$ and $m_{b}$. See [46] for a derivation using twisted mass quarks.

Here we have used the cases $m_{a}=m_{b}$ and both equal to either $m_{l}$ or $m_{s}$ but we can derive from Eq. (A6) a relationship [26] between correlators for the mixed Goldstone pseudoscalar made of light and strange quarks and the 'diagonal' cases:

$$
\begin{align*}
\left(a m_{l}+a m_{s}\right) \sum_{t} C_{K}(t) & =\left(a m_{l}\right) \sum_{t} C_{\pi}(t) \\
& +\left(a m_{s}\right) \sum_{t} C_{\eta_{s}}(t) \tag{A7}
\end{align*}
$$

The left-hand side is then related to the sum of quark masses multiplied by the sum of quark condensates. This does not add new information so we do not make use of this relationship except as a test of our correlators.

## Appendix B: Condensates and the OPE

Condensates typically arise in the non-leading terms of operator-product expansions (OPE). To illustrate, consider moments of two pseudoscalar densities composed of a heavy quark (mass $M$ ) and a light quark (mass $m \ll$ $M)$ where the heavy quark fields are contracted with each other:

$$
\begin{equation*}
(m+M)^{2} \int d \mathbf{x} d t t^{n} J_{5}(\mathbf{x}, t) J_{5}(0) \rightarrow \mathcal{O}^{(n)} \tag{B1}
\end{equation*}
$$

where

$$
\begin{equation*}
\mathcal{O}^{(n)} \equiv \int d \mathbf{x} d t t^{n} \bar{\psi}(\mathbf{x}, t) \gamma_{5} \frac{(m+M)^{2}}{D \cdot \gamma+M} \gamma_{5} \psi(0) \tag{B2}
\end{equation*}
$$

and $\psi$ is the light-quark field. Lattice simulations of $\langle 0| \mathcal{O}^{(n)}|0\rangle$ can be used to determine the heavy quark's mass 47. The $(m+M)^{2}$ factor makes $\mathcal{O}^{(n)}$ independent of the ultraviolet regulator provided $n \geq 4$; that is, lattice and continuum calculations should agree in the limit of zero lattice spacing.

Operator $\mathcal{O}^{(n)}$ is also short-distance, dominated by length scales of order $1 / M$, provided the heavy-quark is sufficiently heavy and the light quarks have momenta small compared with $M$. Consequently the OPE implies that $\mathcal{O}^{(n)}$ can be expressed in terms of a set of local operators in an effective theory, with cutoff scale $\Lambda<M$, and coefficient functions that depend only upon physics between scales $\Lambda$ and $M$ :

$$
\begin{align*}
\bar{M}^{n-4} \mathcal{O}^{(n)} & =\mathbf{1}^{(\Lambda)} c\left(\Lambda / \bar{M}, \bar{\alpha}_{s}, \bar{m} / \bar{M}\right) \\
& +\frac{(m \bar{\psi} \psi)^{(\Lambda)}}{\bar{m} \bar{M}^{3}} d\left(\Lambda / \bar{M}, \bar{\alpha}_{s}, \bar{m} / \bar{M}\right)  \tag{B3}\\
& +\cdots .
\end{align*}
$$

where $\mathbf{1}^{(\Lambda)}$ is the unit operator and we have replaced $\bar{\psi} \psi$ by $m \bar{\psi} \psi$, to simplify the coefficient function. Somewhat arbitrarily, we have chosen to express the right-hand side in terms of masses and couplings at scale $\mu=M(\mu) \equiv \bar{M}$ :

$$
\begin{equation*}
\bar{M} \equiv M(\bar{M}), \quad \bar{m} \equiv m(\bar{M}), \quad \bar{\alpha}_{s} \equiv \alpha_{s}(\bar{M}) \tag{B4}
\end{equation*}
$$

The effective theory on the right-hand side of Eq. (B3) could be, for example, lattice QCD with a lattice spacing $a=\pi / \Lambda$, or QCD with an $\overline{\mathrm{MS}}$ regulator and $\mu=\Lambda$.

The coefficient functions $c$ and $d$ are perturbative when $M$ is large, and analytic in $\bar{\alpha}_{s}$ and $\bar{m} / \bar{M}^{2}$. They can be computed using perturbative matching. For example, we can examine matrix elements of Eq. (B3) between low-energy, on-shell light-quark states $\langle q|$ and $\left|q^{\prime}\right\rangle$. The unit operator drops out and Eq. (B3) can be rearranged to give

$$
\begin{equation*}
d\left(\Lambda / \bar{M}, \bar{\alpha}_{s}, \bar{m} / \bar{M}\right)=\left(\frac{\bar{m} \bar{M}^{n-1}\langle q| \mathcal{O}^{(n)}\left|q^{\prime}\right\rangle}{\langle q| m \bar{\psi} \psi\left|q^{\prime}\right\rangle^{(\Lambda)}}\right)_{\mathrm{PQCD}} \tag{B5}
\end{equation*}
$$

where the right-hand side is computed order-by-order in perturbation theory. Since $\langle q| M \bar{\psi} \psi\left|q^{\prime}\right\rangle$ is independent of $\Lambda, d$ is actually regulator independent:

$$
\begin{equation*}
d=d\left(\bar{\alpha}_{s}, \bar{m} / \bar{M}\right) \tag{B6}
\end{equation*}
$$

Knowing $d$, one would then compute $c$ using perturbative expansions of the vacuum expectation values:

$$
\begin{align*}
& c\left(\Lambda / \bar{M}, \bar{\alpha}_{s}, \bar{m} / \bar{M}\right)= \\
& \quad\left(\frac{\langle 0| \mathcal{O}^{(n)}|0\rangle}{\bar{M}^{4-n}}-\frac{\langle 0| m \bar{\psi} \psi|0\rangle^{(\Lambda)}}{\bar{m} \bar{M}^{3}} d\left(\bar{\alpha}_{s}, \bar{m} / \bar{M}\right)\right)_{\mathrm{PQCD}} \tag{B7}
\end{align*}
$$

Eq. (B7) underscores the importance of avoiding normal-ordered operators in operator-product expansions. Each term on the right-hand side has infrared sensitive contributions that go like $m^{3} \log (m)$. These cancel between the two terms in Eq. (B7), order-by-order in perturbation theory; but this cancelation would have been ruined had we replaced $\bar{\psi} \psi$ by the normal-ordered product : $\bar{\psi} \psi$ : in Eq. B3 (and $c$ would no longer be perturbative).

It is also important to note that $\langle 0| m \bar{\psi} \psi|0\rangle^{(\Lambda)}$ is not cutoff independent, because of operator mixing with the unit operator $m^{4} \mathbf{1}$, which implies that

$$
\begin{equation*}
\frac{d\langle 0| m \bar{\psi} \psi|0\rangle^{(\Lambda)}}{d \log \Lambda}=\gamma_{\text {mix }}\left(\alpha_{s}(\Lambda), m(\Lambda) / \Lambda\right) m^{4}(\Lambda) \tag{B8}
\end{equation*}
$$

where

$$
\begin{equation*}
\gamma_{\mathrm{mix}}\left(\alpha_{s}\right)=\frac{3}{2 \pi^{2}}+O\left(\alpha_{s}\right) \tag{B9}
\end{equation*}
$$

[^307]depends upon the regulator scheme beyond tree-level. This evolution is typically negligible for light quarks because of the $m^{4}$ factor.

## Appendix C: $\overline{\mathrm{MS}}$ condensates from the lattice

The coefficient functions in operator-product expansions such as Eq. ( B 3 ) are most conveniently computed using the $\overline{\mathrm{MS}}$ regulator to define the operators on the right-hand side. On the other hand, the only technology available for determining the nonperturbative matrix elements needed in such analyses is lattice simulation, using the lattice ultraviolet regulator. To combine these techniques we must be able to convert lattice determinations of $\langle 0| m \bar{\psi} \psi|0\rangle$, for example, into the equivalent $\overline{\mathrm{MS}}$ matrix elements.

The relationship is again given by the operator product expansion:

$$
\begin{align*}
(m \bar{\psi} \psi) \frac{(\mu)}{\mathrm{MS}}= & \mathbf{1}^{(a)} \frac{m^{2}}{a^{2}} f(\mu \leftrightarrow \pi / a) \\
& +(m \bar{\psi} \psi)_{\mathrm{LQCD}}^{(a)} h(\mu \leftrightarrow \pi / a)+\cdots \tag{C1}
\end{align*}
$$

where the coefficient functions $f$ and $h$ can only depend upon physics between $\mu$ and the lattice cutoff $\pi / a$. In fact $h=1$ since the matrix elements in

$$
\begin{equation*}
h=\frac{\langle q| m \bar{\psi} \psi\left|q^{\prime}\right\rangle \frac{(\mu)}{\mathrm{MS}}}{\langle q| m \bar{\psi} \psi\left|q^{\prime}\right\rangle_{\mathrm{LQCD}}^{(a)}}=1 \tag{C2}
\end{equation*}
$$

are $\mu$ and $a$ independent, and therefore $h$ must be a number (and 1 is the correct number, from perturbation theory). The coefficient function $f$ is computed order-byorder in perturbation theory using the expansions of the two condensates (computed with their respective regulators):

$$
\begin{align*}
f \equiv & \frac{a^{2}}{m^{2}}\left(\langle 0| m \bar{\psi} \psi|0\rangle \frac{(\mu)}{\mathrm{MS}}-\langle 0| m \bar{\psi} \psi|0\rangle_{\mathrm{LQCD}}^{(a)}\right)_{\mathrm{PQCD}} \\
= & \sum_{n=0} f_{n}^{(0)}(a \mu) \alpha_{\overline{\mathrm{MS}}}^{n}(\mu) \\
& +(a m)^{2} \sum_{n=0} f_{n}^{(1)}(a \mu) \alpha_{\overline{\mathrm{MS}}}^{n}(\mu) \tag{C3}
\end{align*}
$$

The cancellation of all $\log m$ terms between the two matrix elements in $f$ is something of a miracle; it only works if the $m$ in each case is precisely the $m$ that multiplies $\bar{\psi} \psi$ in the action for that case ${ }^{3} . \Delta_{P T}$ in eq. $(21)$ is $(a m)^{2} f$ calculated through $\mathcal{O}\left(\alpha_{s}\right)$.

Additional terms appear in Eq. C1 from mixing with higher dimension condensates, such as the gluon condensate. These are suppressed by positive powers of $a$. For

[^308]the gluon condensate the multiplier is $(m a)^{2}$ from chirality arguments. These terms then simply look like discretisation errors in $m \bar{\psi} \psi$ and are handed as part of the general treatment of those errors.

## Appendix D: Lattice QCD calculation on $n_{f}=2+1$ gluon configurations

We show here further results for the strange quark condensate from two contrasting calculations, both using HISQ quarks, that include $u, d$ and $s$ quarks in the sea, but no $c$ quarks. The first calculation uses sets of MILC configurations corresponding to 5 values of lattice spacing spanning a large range from 0.15 fm to 0.04 fm [48] and using the asqtad formalism for the sea quarks. The second uses HOTQCD configurations [35] and has more lattice spacing values ( 24 in total) but with only a limited number (9) having accompanying meson masses and decay constants. The sea quarks are included using the HISQ formalism with $u / d$ sea quark masses close to the physical value. The second calculation corresponds to the zero temperature results generated to accompany a finite temperature analysis of the phase structure of QCD. This analysis needs many values of the lattice spacing for a fine-grained temperature scale, and the zero temperature results are needed to fix the QCD parameters. The quark condensate is an important order parameter at finite temperature but is also determined in [35] on the zero temperature ensembles.

For the first calculation we use values of the strange quark condensate listed in Table VI. These are obtained from studies of the $\eta_{s}$ correlator on 9 different ensembles at 5 different values of the lattice spacing and multiple sea quark mass values. The lattice spacing values we use here are defined from the $\eta_{s}$ decay constant and are determined in 48. From the values in Table VI we can construct the ratio $R_{s}$ defined in Eq. (24) and fit it as a function of lattice spacing in exactly the same way as that described in section III B 2. The $\mathcal{O}\left(\alpha_{s}^{0}\right)$ and $\mathcal{O}\left(\alpha_{s}^{1}\right)$ perturbative subtractions defined in section III A apply here also since no effects appear at this order from the differing number of sea quarks or the formalism used for them or the improvement coefficients in the gluon action (the MILC $2+1$ asqtad configurations do not include the $n_{f} \alpha_{s} a^{2}$ improvement coefficients in the gluon action). These effects will cause differences in the perturbation theory at $\mathcal{O}\left(\alpha_{s}^{2}\right)$. The $\alpha_{s}^{2}$ and higher order divergent pieces of the condensate are included in the fit with coefficients that, as before, are given a prior value of $0(4)$. The appropriate $\alpha_{s}$ value in this case is $\alpha_{V}^{n_{f}=3}(2 / a)$ rather than $\alpha_{V}^{n_{f}=4}(2 / a)$. Multiple valence $s$ quark masses are given at each lattice spacing and we allow for linear and quadratic dependence on the mistuning of the $s$ quark mass, again as described in section III B 2. We allow for mistuning of the sea quark masses through use of the parameter $\delta x_{\text {sea }}$ 49].


FIG. 12: Results from fitting the values for $R_{s}$ obtained on MILC configurations including $2+1$ flavors of asqtad sea quarks, as described in the text. The crosses give the calculated values after perturbative subtraction through $\mathcal{O}\left(\alpha_{s}\right)$. The hatched band corresponds to the fitted physical value after removing the remaining power divergence and discretisation and sea quark mass effects. Compare to Fig. 6 which includes $2+1+1$ flavors of HISQ sea quarks.

Figure 12 shows, as a hatched band, the physical result from the fit, which has $\chi^{2} /$ dof $=0.4$ for 20 degrees of freedom. For comparison the data points given are the values after perturbative subtraction through $\mathcal{O}\left(\alpha_{s}\right)$. The physical value obtained is

$$
\begin{equation*}
R_{s, p h y s}=0.555(84) \tag{D1}
\end{equation*}
$$

This is completely consistent with the result from $2+1+1$ flavors of HISQ sea quarks in section IIIB 2, and has a similar error. It is not such a complete calculation, lacking light quark mass results and not having such light sea quark masses, and is therefore not our preferred final result. It provides a strong check of our $2+1+1$ result, however, being a completely independent set of numbers. The fits to the $2+1$ results give very similar behaviour to that seen for the $2+1+1$ case, for example choosing a coefficient of the $\alpha_{s}^{2} / a^{2}$ divergence of around 2 .

For the second calculation we use values of the strange condensate from the HOTQCD collaboration [35]. They generated ensembles with an improved gluon action and $u / d$ and $s$ quarks in the sea using the HISQ formalism. The QCD action differs slightly from that in section III. Apart from missing $c$ quarks in the sea, the gauge field configurations here are improved through $\mathcal{O}\left(a^{2}\right)$ at treelevel and without tadpole-improvement, i.e. the fairly substantial $\mathcal{O}\left(\alpha_{s} a^{2}\right)$ improvement coefficients were not included. The lattice spacing was determined using the $r_{1}$ heavy quark potential parameter, or $r_{0}$ on the coarsest lattices where $r_{1} / a<2$. The $s$ quark mass was tuned by determining the mass of the $\eta_{s}$ meson and the light

TABLE VI: Raw (unsubtracted) values for the strange quark condensate along with $\eta_{s}$ masses and decay constants in lattice units calculated for valence masses given in column 4. The calculations use valence HISQ quarks on MILC configuration sets labelled in column 1 that include $2+1$ flavors of asqtad quarks (see 48 for more details about the ensembles). The results are derived from the correlators calculated in [48] and 49] along with Eq.(11), but we also give results for additional strange quark masses on sets 1 and $2 . \delta x_{\text {sea }}$ is the mismatch between the sea $2 m_{l}+m_{s}$ value and the physical result divided by the physical value of $m_{s}$ 49].

| Set | $\delta x_{s e a}$ | $a_{\eta_{s}}(\mathrm{fm})$ | $a m_{s, v a l}$ | $a M_{\eta_{s}}$ | $a f_{\eta_{s}}$ | ${ }_{-} a^{3}\left\langle\bar{\psi} \psi_{s}\right\rangle_{0}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0.47 | 0.1583(13) | 0.061 | 0.50490(36) | 0.1410(4) | 0.042399(38) |
|  |  |  | 0.066 | 0.52524(36) | 0.1429(4) | 0.044637(38) |
|  |  |  | 0.080 | 0.57828(34) | 0.1485(4) | 0.050795(37) |
| 2 | 0.91 | 0.1595(14) | 0.066 | 0.52458(35) | 0.1434(3) | 0.044714(37) |
| 3 | 0.64 | $0.1247(10)$ | 0.0489 | 0.41133(17) | 0.1124(2) | 0.030233(14) |
|  |  |  | 0.0537 | 0.4310(4) | 0.1144(2) | 0.032423(15) |
| 4 | 0.93 | $0.1264(11)$ | 0.0492 | 0.41436(23) | 0.1136(2) | 0.030585(21) |
|  |  |  | 0.0546 | $0.43654(24)$ | 0.1160(3) | 0.033041(20) |
|  |  |  | 0.060 | 0.45787(23) | 0.1182(4) | 0.035476(20) |
| 5 | 1.5 | 0.1263(11) | 0.0491 | 0.41196(24) | 0.1135(2) | 0.030306(21) |
|  |  |  | 0.0525 | 0.4259(6) | 0.1149(4) | 0.031817(23) |
|  |  |  | 0.0556 | 0.4384(6) | 0.1161(4) | 0.033211(23) |
| 6 | 0.59 | 0.0878(7) | 0.0337 | 0.29413(12) | 0.07954(9) | 0.018310(5) |
|  |  |  | 0.0358 | 0.30332(12) | 0.08051(9) | 0.019273(5) |
|  |  |  | 0.0382 | 0.31362(14) | 0.08171(15) | 0.020370(5) |
| 7 | 1.1 | 0.0884(7) | 0.0336 | 0.29309(13) | 0.07959(11) | 0.018217(5) |
|  |  |  | 0.03635 | 0.30513(20) | 0.08095(14) | 0.019467(7) |
| 8 | 0.28 | 0.0601(5) | 0.0228 | 0.20621(19) | 0.0549(2) | 0.011311(5) |
|  |  |  | 0.024 | 0.21196(13) | 0.0556(1) | 0.011851(3) |
| 9 | 0.38 | 0.0443(4) | 0.0161 | 0.1525(2) | 0.0404(1) | 0.0075891(20) |

quark mass was taken as $m_{s} / 20$ (with some values available for $m_{s} / 5$ but we have not used those). Results for the zero temperature strange condensate are available at 24 values of the lattice spacing from 0.2 fm to 0.07 fm (Table 14 of 35 ] gives values for two times the condensate). Note that these results were obtained by direct calculation of $\left\langle\operatorname{Tr} M^{-1}\right\rangle$ using stochastic techniques. Corresponding values of the lattice spacing are given in Table 16 of [35]; some missing values can be inferred from the tables of temperature values at the corresponding value of $\beta$.

Figure 13 shows the raw unsubtracted results for $m_{s}\left\langle\bar{\psi} \psi_{s}\right\rangle$ as a function of the square of the inverse lattice spacing, as well as the values after making the complete subtraction through $\mathcal{O}\left(\alpha_{s}\right)$ as given in Eq. 21). As for $R_{s}$ in section III B 1 (Fig. 4), the unsubtracted results show clear evidence of a quadratic term in $a^{-1}$ which is significantly reduced, but not completely absent, after the perturbative subtraction.

For a subset of 9 lattice spacing values meson masses and decay constants are also given in Tables 18 and 19 of 35. In fact we use the 7 finest values only because the $s$ quark mass is not as well-tuned for our purposes on the coarsest two lattices. Note that the decay constant values need to be multiplied by $\sqrt{2}$ to match the convention used here. For these we can construct the ratio $R_{s}$ given in 24 . To obtain a physical result for $R_{s}$ we fit the subtracted


FIG. 13: Bursts give the raw data for $m_{s}\left\langle\bar{\psi} \psi_{s}\right\rangle$ from 35 as a function of the square of the inverse lattice spacing. Open circles give results after subtraction of the $\mathcal{O}\left(\alpha_{s}\right)$ perturbative contribution.
results as a function of lattice spacing in the same way as in section III B 2, apart from the use of $\alpha_{V}^{n_{f}=3}(2 / a)$ rather than $\alpha_{V}^{n_{f}=4}(2 / a)$.

The physical value for $R_{s}$ obtained from the fit is

$$
\begin{equation*}
R_{s}=0.79(34) \tag{D2}
\end{equation*}
$$

This is much less accurate than the result from section III, but agrees both with that and the result from
the MILC $2+1$ asqtad ensembles given earlier in this section. We have not extracted a light quark condensate from the HOTQCD results because finite volume sensitivity obscures the power divergence and leads to larger errors.

We conclude from this that there is no sign of disagreeement between the strange quark condensate extracted with $u, d$ and $s$ quarks in the sea and those including also $c$ quarks in the sea.
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[^14]:    2 The limits presented in this study for $m_{H}>200 \mathrm{GeV}$ assume cross sections based on on-shell Higgs boson production and decay and use MC generators with an ad hoc Breit-Wigner Higgs line shape. Recently potentially important effects related to off-shell Higgs boson production and interference effects between the Higgs boson signal and backgrounds have been discussed $[17,45]$. The inclusion of such effects may affect limits at high Higgs masses ( $m_{H}>400 \mathrm{GeV}$ ).

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[^16]:    2 See footnote 1.

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[^23]:    ${ }^{1}$ The symbol $\ell$ stands for electron or muon.

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[^25]:    ${ }^{3} p_{\mathrm{Tt}}=\left|\left(\mathbf{p}_{\mathrm{T}}^{\gamma_{1}}+\mathbf{p}_{\mathrm{T}}^{\gamma_{2}}\right) \times\left(\mathbf{p}_{\mathrm{T}}^{\gamma_{1}}-\mathbf{p}_{\mathrm{T}}^{\gamma_{2}}\right)\right| /\left|\mathbf{p}_{\mathrm{T}}^{\gamma_{1}}-\mathbf{p}_{\mathrm{T}}^{\gamma_{2}}\right|$, where $\mathbf{p}_{\mathrm{T}}^{\gamma_{1}}$ and $\mathbf{p}_{\mathrm{T}}^{\gamma_{2}}$ are the transverse momenta of the two photons.

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[^40]:    ${ }^{1}$ In this paper, the raised index '*' implies a particle off mass-shell, $\ell$ is always taken to mean either $e$ or $\mu$ and $q$ can be any of $u, d, s, c$ or $b$.

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[^42]:    ${ }^{2}$ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the

[^43]:    $z$-axis coinciding with the axis of the beam pipe. The $x$-axis points from the IP to the centre of the LHC ring, and the $y$-axis points upward. Cylindrical coordinates $(r, \phi)$ are used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta=-\ln \tan (\theta / 2)$.

[^44]:    ${ }^{3}$ When two errors are quoted the first is statistical and the second systematic.

[^45]:    ${ }^{4}$ In this channel the jet $p_{\text {T }}$ threshold is raised from 25 GeV to 30 GeV .

[^46]:    ${ }^{1}$ In the following, charged Higgs bosons are denoted $H^{+}$, with the charge-conjugate $H^{-}$always implied. Hence, $\tau$ denotes a positively charged $\tau$ lepton.

[^47]:    ${ }^{2}$ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the $z$-axis along the beam pipe. The $x$-axis points from the IP to the centre of the LHC ring, and the $y$-axis points upwards. Cylindrical coordinates $(r, \phi)$ are used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta=-\ln \tan (\theta / 2)$.

[^48]:    ${ }^{3} \Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}$, where $\Delta \eta$ is the difference in pseudorapidity of the two objects in question, and $\Delta \phi$ is the difference between their azimuthal angles.

[^49]:    ${ }^{4}$ The electron trigger threshold was increased from 20 GeV to 22 GeV towards the end of data-taking in 2011.

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[^53]:    ${ }^{1} w_{\eta^{2}}$ is defined as $\sqrt{\frac{\sum E_{i} \eta_{i}^{2}}{\sum E_{i}}-\left(\frac{\sum E_{i} \eta_{i}}{\sum E_{i}}\right)^{2}}$, where the sums are computed using all the cells $i$ of the cluster ( $E_{i}$ is the energy released in the cell and $\eta_{i}$ its pseudorapidity).

[^54]:    ${ }^{2}$ This uncertainty is mainly due to uncertainties in the transport of the electromagnetic scale determined in the test-beams to the ATLAS detector. For the electromagnetic calorimeter this uncertainty will be much reduced when a sufficient number of $Z$ bosons decaying to electrons is available.

[^55]:    ${ }^{1}$ The ATLAS Coordinate System is a right-handed system with the $x$-axis pointing to the centre of the LHC ring, the $z$-axis following the beam direction and the $y$-axis pointing upwards. The pseudorapidity $\eta$ is an approximation for rapidity $y$ in the high energy limit, and it is related to the polar angle $\theta$ as $\eta=-\ln \tan \frac{\theta}{2}$.

[^56]:    ${ }^{2}$ This additional calibration has been applied to the electromagnetic barrel, electromagnetic endcap and to the full forward calorimeter.

[^57]:    ${ }^{3}$ The truth isolation cut on the average jet response has a negligible impact on the average jet response.

[^58]:    ${ }^{4}$ Time-dependent noise changes for single cells in data are accounted for using regular measurements.

[^59]:    ${ }^{1}$ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector and the $z$-axis along the beam pipe. The $x$-axis points from the IP to the centre of the LHC ring, and the $y$ axis points upward. Cylindrical coordinates $(r, \phi)$ are used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta=-\ln \tan (\theta / 2)$.

[^60]:    ${ }^{1}$ Hereafter the charged Higgs bosons will be denoted $H^{+}$, with the charge-conjugate processes implied.

[^61]:    ${ }^{2} \Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}$, where $\eta$ is the pseudorapidity and $\phi$ the azimuthal angle.

[^62]:    ${ }^{1}$ ATLAS uses a right-handed coordinate system originated at the nominal interaction point. The z -axis is along the beam pipe, the $x$-axis points to the centre of the LHC ring and the $y$-axis points upward. Cylindrical coordinates ( $\mathrm{r}, \phi$ ) are used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudorapidity $\eta$ is defined as $\eta=-\ln [\tan (\theta / 2)]$ where $\theta$ is the polar angle.

[^63]:    ${ }^{2}$ The limits presented in this search assume cross sections based on on-shell Higgs boson production and decay and use MC generators with an ad-hoc Breit-Wigner Higgs line shape. Recently potentially important effects related to off-shell Higgs boson production and interference effects between the Higgs boson signal and backgrounds have been discussed [17,48]. The inclusion of such effect may affect limits at very high Higgs masses ( $m_{H}>400 \mathrm{GeV}$ ).

[^64]:    ${ }^{1}$ Hereafter the charged Higgs bosons will be denoted $H^{+}$, with the charge-conjugate $H^{-}$always implied.

[^65]:    ${ }^{2} \Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}$, where $\Delta \eta$ is the difference in pseudorapitidy of the two objects in question, and $\Delta \phi$ the difference of their azimuthal angles.

[^66]:    ${ }^{1}$ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the center of the detector and the z -axis along the beam pipe. The x -axis points from the IP to the center of the LHC ring, and the y axis points upward. Cylindrical coordinates $(\mathrm{R}, \phi)$ are used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta=-\ln \tan (\theta / 2)$.

[^67]:    ${ }^{1}$ The kinematic acceptance of this search has not been optimized for low mass Higgs bosons.
    ${ }^{2}$ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point. The $z$-axis is along the beam pipe, the $x$-axis points to the centre of the LHC ring and the $y$-axis points upward. Cylindrical coordinates ( $\mathrm{r}, \phi$ ) are used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudorapidity $\eta$ is defined as $\eta=-\ln [\tan (\theta / 2)]$ where $\theta$ is the polar angle.

[^68]:    ${ }^{1}$ ATLAS uses a right-handed coordinate system with the $z$-axis along the beam pipe. The $x$-axis points to the center of the LHC ring, and the $y$ axis points upward. Cylindrical coordinates $(r, \phi)$ are used in the transverse plane, $\phi$ being the azimuthal angle. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta=-\ln \tan (\theta / 2)$.

[^69]:    ${ }^{1}$ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point. The $z$-axis is along the beam pipe, the $x$-axis points to the centre of the LHC ring and the $y$-axis is defined as pointing upwards. Polar coordinates $(r, \phi)$ are used in the transverse plane, $\phi$ being the azimuthal angle around the beam pipe. The pseudo-rapidity $\eta$ is defined as $\eta=-\ln [\tan (\theta / 2)]$ where $\theta$ is the polar angle.

[^70]:    ${ }^{1}$ ATLAS uses a right-handed coordinate system with its origin at the nominal interaction point (IP) in the centre of the detector, and the $z$-axis along the beam line. The $x$-axis points from the IP to the centre of the LHC ring, and the $y$-axis points upwards. Cylindrical coordinates $(r, \phi)$ are used in the transverse plane, $\phi$ being the azimuthal angle around the beam line. The pseudorapidity is defined in terms of the polar angle $\theta$ as $\eta=-\ln \tan (\theta / 2)$.

[^71]:    ${ }^{1}$ Hereafter the charged Higgs bosons will be denoted $H^{+}$, with the charge-conjugate $H^{-}$always implied.

[^72]:    ${ }^{2} \Delta R=\sqrt{(\Delta \eta)^{2}+(\Delta \phi)^{2}}$, where $\Delta \eta$ is the difference in pseudorapitidy of the two objects in question, and $\Delta \phi$ the difference of their azimuthal angles.

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[^80]:    ${ }^{1}$ The details of this definition are outlined in Refs. [16,17]. While we focus on $F_{2}$, we can consider other observables such as $\left\{F_{1}, F_{3}, d \sigma\right\}$ in a similar manner.

[^81]:    ${ }^{2}$ Note that the Ucor5 fit improves the average $\chi^{2} / p t$ at the expense of an increased $\chi^{2} / p t$ for particular data sets; this reflects the tension (and the different number of data points) between the $\ell^{ \pm} A$ and $\nu A$ data sets.
    ${ }^{3}$ For $x<0.4, \mathrm{NuTeV}$ is compatible with both CCFR and CDHSW data; for larger $x, \mathrm{NuTeV}$ agrees with CDHSW, and the difference with CCFR has been reconciled.

[^82]:    *Presented by Fred Olness

[^83]:    ${ }^{2}$ While the nuclear PDFs can be finite for $x>1$, the magnitude of the PDFs in this region is negligible for the purposes of the present study (cf., Refs. [6, 7, 8, 9, 10]).

[^84]:    ${ }^{3}$ Cf. the Durham HEP Databases for a complete listing: http://www-spires.dur.ac.uk/hepdata/

[^85]:    ${ }^{4}$ We do retain the deuteron data as this has only a small correction over the central $x$-range [3, 1]. The deuteron correction has been applied in the Base-1 fit. Also, for the Drell-Yan Cu data (E605), the expected nuclear corrections in this kinematic range are small (a few percent) compared to the overall normalization uncertainty ( $15 \%$ ) and systematic error ( $10 \%$ ).
    ${ }^{5}$ These PDFs have been determined from a fit to the same data set as in the CTEQ6 analysis with the addition of the the NuTeV dimuon data. The changes to the strange sea induce only minor changes to the other fit parameters; this has a minimal effect on the particular observables ( $d \sigma$, $F_{2}$ ) we examine in the present study.

[^86]:    ${ }^{6}$ While iron is roughly isoscalar, other nuclear PDFs can exhibit larger differences between the $u$ and $d$ distributions-the extreme case being the free-proton PDF. When comparing PDFs we must keep in mind that it is ultimately the structure functions which are the physical observables.
    ${ }^{7}$ In a recent publication, Eskola et al. [10] perform a global reanalysis of their ESK98 [9] nuclear PDFs. While we do not present a comparison here, the results are compatible with those distributions displayed in Fig. 1; a comparison can be found in Figs. 10 and 11 of Ref. [10].

[^87]:    ${ }^{8}$ The corresponding anti-neutrino process is obtained with a $u \leftrightarrow d$ interchange.
    ${ }^{9}$ Note that our comparison with the Kulagin-Petti model is based on the work in Ref. [28].

[^88]:    ${ }^{10}$ In particular, we will find for large $x(\gtrsim 0.5)$ and $Q$ comparable to the proton mass the target mass corrections for $F_{2}^{\mathrm{Fe}} / F_{2}^{\mathrm{D}}$ are essential for reproducing the features of the data; hence the $Q$ dependence plays a fundamental role.

[^89]:    ${ }^{11}$ In Ref. [39], Brodsky and collaborators posit a nonuniversal nuclear anti-shadowing mechanism which yields different effects for CC and NC scattering.

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[^91]:    ${ }^{1}$ Technically, the heavy-target data were scaled to a deuteron target, and then isospin symmetry relations were used to obtain the corresponding proton data. Deuteron corrections were used in certain cases.

[^92]:    ${ }^{2}$ The nuclear analogue of the scaling variable $x$ is defined as $x:=A x_{A}$, where $x_{A}=Q^{2} / 2 P_{A} \cdot q$ is the usual Bjorken variable formed out of the four-momenta of the nucleus $\left(P_{A}\right)$ and the exchanged boson $(q)$, with $Q^{2}=-q^{2}$ [33].

[^93]:    ${ }^{3}$ For example, see the CTEQ (Coordinated TheoreticalExperimental Project on QCD) analysis of Ref. [34] which presents the CTEQ6 PDF sets.

[^94]:    ${ }^{4}$ While Ref. [33] extracted the nuclear PDFs using only the NuTeV neutrino-iron DIS data, Ref. [30] demonstrated that the Chorus neutrino-lead DIS data [52] was consistent with the NuTeV data set.

[^95]:    ${ }^{5}$ While it is straightforward to obtain a "fit" to the combined neutrino and charged-lepton DIS data sets, determining the appropriate weights of the various sets and discerning whether this compromise fit is within the allowable uncertainty range of the data is a more involved task. This work is presently ongoing.

[^96]:    ${ }^{1}$ Presented by F. Olness.

[^97]:    ${ }^{2}$ The nuclear PDFs are available on the web from the nCTEQ page at http://projects.hepforge.org/ncteq/ which is hosted by the HepForge project.

[^98]:    ${ }^{3}$ Cf., ZEUS-prel-09-015

[^99]:    ${ }^{4}$ Specifically, the $\chi$-prescription rescales the partonic momentum fraction via $x \rightarrow x\left(1+\left(2 m_{c} / Q\right)^{2}\right)$ in contrast to the traditional Barnett [29] "slow-rescaling" which is $x \rightarrow x\left(1+\left(m_{c} / Q\right)^{2}\right)$.

[^100]:    ${ }^{5}$ For details, c.f., Refs. [30, 31]

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[^105]:    ${ }^{1}$ The one exception is the CCFR $F_{2}$ which is mildly sensitive to the strange quark PDF via Eq. (1).

[^106]:    ${ }^{2}$ In Eq. (5), $X$ is the observable, $S_{i}^{ \pm}$are the error PDF sets for eigenvalue $i$, and $N_{p}$ is the number of eigenvalues. For CTEQ6.5 $N_{p}=20$, and for CTEQ6.6 $N_{p}=22$.

[^107]:    ${ }^{3}$ Here, we are more interested in the general span of these different PDFs rather than the specific sets and values. For reference, reading from the top to bottom (at $y=0$ ) in Fig. 9(c) left ( $W^{-}$), the specific curves are ABKM09 [22] (gray), MSTW2008 [20] (magenta), HERAPDF10 [72] (orange), CT10 [70] (purple), CTEQ6.5 [71] (black), NNPDF [69] (blue), MRST2004 [73] (red), CTEQ6.1 [18] (green).

[^108]:    ${ }^{4}$ We follow the methodology and notation of Ref. [27]. See this reference for details.

[^109]:    *Presented by Fred Olness

[^110]:    ${ }^{2}$ While we have given a heuristic description of this result (in which we used some illustrative approximations), we emphasize the proof applies to all cases and does not require any such approximations.

[^111]:    ${ }^{3}$ Specifically, ACOT was used for CTEQ6HQ, and S-ACOT- $\chi$ was used in CTEQ6.5 and CTEQ6.6.

[^112]:    ${ }^{4}$ Here, we define the order of the calculation according to the power of $\alpha_{S}$; thus LO is $\alpha_{s}^{0}$, NLO is $\alpha_{s}^{1}$, etc.

[^113]:    ${ }^{5}$ Note, in Figure 7 and in the discussion the diagrams an processes are schematic and illustrative. For example, at NLO we include both $\gamma Q \rightarrow Q g$ and $\gamma g \rightarrow Q \bar{Q}$ as well as all the corresponding subtractions. For details see Refs. [ $22,24]$.

[^114]:    ${ }^{6}$ Recall $\alpha_{S}(\mu)$ is also an unphysical theoretical construct; this has discontinuities across flavor-thresholds at order $\alpha_{s}^{3}$.

[^115]:    ${ }^{7}$ The matching conditions are determined entirely by the DGLAP evolution kernels up to a constant term which must be computed. At NLO, the constant term is zero such that the PDFs are continuous; at NNLO, this term is non-zero.

[^116]:    ${ }^{1}$ Contributed by: J. Fleischer, T. Riemann, V. Yundin
    ${ }^{2}$ An extended description of notations and of the formalism may be found in [105, 106, 107, 108]. The normalization of PJFry follows that chosen in the scalar library. For QCDLoop, $C(\epsilon)=\Gamma(1-2 \epsilon) /\left[\Gamma(1+\epsilon) \Gamma^{2}(1-\epsilon)\right]$.

[^117]:    ${ }^{3}$ One has to carefully control accuracies; e.g. the on-shell conditions for massless particles have to be fulfilled with a numerical precision expected by the scalar functions library in use; for QCDLoop this means on default at least 10 digits.

[^118]:    ${ }^{4}$ Contributed by: G. Cullen, N. Greiner, G. Heinrich, G. Luisoni, P. Mastrolia, G. Ossola, T. Reiter, F. Tramontano

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[^125]:    ${ }^{11}$ Contributed by: T. Stavreva, I. Schienbein, F. I. Olness, T. Ježo, K. Kovařík, A. Kusina, J. Y. Yu

[^126]:    ${ }^{12}$ There has been a calculation of neutral current electroproduction of heavy quarks $\mathcal{O}\left(\alpha_{s}^{2}\right)$ in the FFNS [326]. however, extra contributions are still required for a VFNS calculation 327.
    ${ }^{13}$ See Ref. [328] and references therein.
    ${ }^{14}$ Details will be presented in a forthcoming publication.
    ${ }^{15}$ Of course, once the massive higher order Wilson coefficients have been computed, it is straightforward to incorporate these results into our calculations.

[^127]:    ${ }^{16}$ Contributed by: A. Denner, S. Dittmaier, S. Kallweit, S. Pozzorini, M. Schulze

[^128]:    ${ }^{17}$ Recent progress in the theoretical description of top-quark pair production at hadron colliders is reviewed in Refs. [332, 333, 334.
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[^166]:    ${ }^{60}$ One could also reconstruct the mass given energy and momentum, but this typically gives large precision problems for small masses.

[^167]:    * Presented by A. Kusina at the Cracow Epiphany Conference on Present and Future of $B$ Physics, Cracow, Poland, January 9-11, 2012.

[^168]:    ${ }^{1}$ Similar considerations also hold for target mass corrections (TMC) and higher twist terms. We focus here mainly on the kinematic region $x<0.1$, where TMC are small [1]. An inclusion of higher twist terms is beyond the scope of this study.

[^169]:    ${ }^{2}$ At NLO, there are corresponding quark-initiated terms; for simplicity we do not display them here, but they are fully contained in our calculations [7].

[^170]:    ${ }^{3}$ Use of more general rescaling prescriptions have been discussed in Ref. [13].

[^171]:    ${ }^{4}$ For the original ACOT scheme it would then still be necessary to compute the massive Wilson coefficients for the heavy quark initiated subprocess at $\mathcal{O}\left(\alpha \alpha_{\mathrm{S}}^{2}\right)$. See Refs. [12, 20] for details.

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[^181]:    ${ }^{4}$ In this subsection we will distinguish $\mu$ and $Q$; in the following, we will set $\mu=Q$ and display the results as a function of $Q$.
    ${ }^{5}$ If we were to compute this process in the $\overline{\mathrm{MS}}$ scheme, the $\ln \left(m^{2} / Q^{2}\right)$ in the SUB term would simply be replaced by a $1 / \varepsilon$ pole which would cancel the corresponding singularity in the NLO contribution.

[^182]:    ${ }^{6}$ It is possible to define other massive schemes that could include additional matching parameters or extra observabledependent contributions. For example, the calculation of $F_{2}^{c}$ in the original RT scheme [7] included extra higher-order contributions that do not vanish as $Q / m \rightarrow \infty$.

[^183]:    ${ }^{7}$ If the beam has nonzero charm-flavor quantum number, such as a $D$-meson, this argument would be incorrect. Technically, $\chi$ scaling violates factorization as we are presuming the mass of the beam fragments; if we perform a thought experiment with a beam of $D$-mesons, charm quark need not be associated with an anticharm quark.
    ${ }^{8}$ We sketch the relevant kinematics in Appendix A.

[^184]:    ${ }^{9}$ Note that the finite mass terms $\left(m^{2} / Q^{2}\right)^{n}$ in $\hat{\sigma}(m)$ receive contributions from both, masses in the heavy quark propagators and masses in the phase space. Still we refer to them as dynamic mass terms and show that they are numerically less important than the mass terms in the slow-rescaling variable $\chi(n)$ which are of purely kinematic origin.

[^185]:    ${ }^{10}$ In Sec. II A 2 we demonstrated that the ACOT calculation reduces to the ZM-VFNS result in the massless limit. We will address the choice of the $\chi(n)$ rescaling in Sec. III A.

[^186]:    ${ }^{11}$ Fractional decomposition of "initial-state" structure functions is understood as $F_{2, L}^{i}=\sum_{j=1}^{6} F_{2, L}^{i j}$.

[^187]:    ${ }^{12}$ Because we use the fully massive ACOT scheme to LO and NLO, the LO result in Fig. 14(b) contains the ( $\mathrm{m}^{2} / Q^{2}$ ) helicityviolating contributions $\sim \mathcal{O}\left(\alpha_{s}^{0}\right)$; hence, it is nonzero. In the S-ACOT scheme, the LO result for $F_{L}$ vanishes, but the NLO result is comparable to the NLO ACOT result.

[^188]:    ${ }^{13}$ Note that in our decomposition, diagrams with a bottom quark in the initial or final state, contribute to the bottom structure function, even in the presence of a charm quark.

[^189]:    ${ }^{14}$ At present, the full set of matching conditions and DGLAP kernels have not been computed at $\mathrm{N}^{3} \mathrm{LO}$.

[^190]:    ${ }^{15}$ Note, we will focus on the gluon-initiated terms, but the demonstration for the quark-initiated pieces is analogous.

[^191]:    ${ }^{16}$ The explicit form of the ACOT subtraction is defined in Sec. IV C [cf. Eq. (36)] of Ref. [5]. For an example of the cancellation between $\sigma_{\mathrm{LO}}$ and $\sigma_{\mathrm{SUB}}$ in a more general context, see Ref. [42].

[^192]:    ${ }^{1}$ Contributed by: J. Fleischer, T. Riemann, V. Yundin
    ${ }^{2}$ An extended description of notations and of the formalism may be found in [105, 106, 107, 108]. The normalization of PJFry follows that chosen in the scalar library. For QCDLoop, $C(\epsilon)=\Gamma(1-2 \epsilon) /\left[\Gamma(1+\epsilon) \Gamma^{2}(1-\epsilon)\right]$.

[^193]:    ${ }^{3}$ One has to carefully control accuracies; e.g. the on-shell conditions for massless particles have to be fulfilled with a numerical precision expected by the scalar functions library in use; for QCDLoop this means on default at least 10 digits.

[^194]:    ${ }^{4}$ Contributed by: G. Cullen, N. Greiner, G. Heinrich, G. Luisoni, P. Mastrolia, G. Ossola, T. Reiter, F. Tramontano

[^195]:    ${ }^{5}$ Contributed by: S. Weinzierl

[^196]:    ${ }^{6}$ Contributed by: F. Campanario

[^197]:    ${ }^{7}$ Contributed by: G. Chachamis

[^198]:    ${ }^{8}$ Contributed by: G. Somogyi, Z. Szőr, Z. Trócsányi

[^199]:    ${ }^{9}$ Contributed by: Z. Liang, P. M. Nadolsky

[^200]:    ${ }^{10}$ Contributed by: R. D. Ball, N. P. Hartland, J. Rojo and M. Ubiali

[^201]:    ${ }^{11}$ Contributed by: T. Stavreva, I. Schienbein, F. I. Olness, T. Ježo, K. Kovařík, A. Kusina, J. Y. Yu

[^202]:    ${ }^{12}$ There has been a calculation of neutral current electroproduction of heavy quarks $\mathcal{O}\left(\alpha_{s}^{2}\right)$ in the FFNS [326]. however, extra contributions are still required for a VFNS calculation 327.
    ${ }^{13}$ See Ref. [328] and references therein.
    ${ }^{14}$ Details will be presented in a forthcoming publication.
    ${ }^{15}$ Of course, once the massive higher order Wilson coefficients have been computed, it is straightforward to incorporate these results into our calculations.

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[^242]:    ${ }^{60}$ One could also reconstruct the mass given energy and momentum, but this typically gives large precision problems for small masses.

[^243]:    ${ }^{1}$ Recently, a paper by Paukkunen and Salgado [20] discussed that weak boson production at the LHC might be useful in order to constrain nPDFs.
    ${ }^{2}$ Note that the EPS08/EPS09 $[14,15]$ global analyses include single-inclusive $\pi^{0}$ data from the PHENIX experiment at RHIC.
    ${ }^{3}$ A recent paper by Betemps and Machado [27] has performed a calculation for $\gamma+c$ production using however the target rest frame formalism.

[^244]:    ${ }^{4}$ We do not distinguish between heavy-quark and heavy-anti-quark in the final state, that is the sum of $\gamma+Q$ and $\gamma+\bar{Q}$ is considered; therefore here by $q Q \rightarrow q Q \gamma$ we choose to denote the sum of $q Q \rightarrow q Q \gamma$, $q \bar{Q} \rightarrow q \bar{Q} \gamma, \bar{q} Q \rightarrow \bar{q} Q \gamma$ and $\bar{q} \bar{Q} \rightarrow \bar{q} \bar{Q} \gamma$.
    ${ }^{5}$ In $p p$ and $p A$ collisions, however, the Compton subprocess largely dominates the annihilation process from the dominance of the gluon distribution over that of sea-quarks.

[^245]:    ${ }^{6}$ Note that the nDS 04 PDFs [12] are not considered here since these are obtained in a 3-fixed flavor number scheme (no charm PDF) whereas our calculation is in a variable flavor number scheme.
    ${ }^{7}$ More precisely, EPS09 is linked to the CTEQ6.1M proton PDFs [34], HKN07 to the MRST98 [35] set, and the nCTEQ PDFs to the reference PDFs described in ref. [36] which are very similar to the CTEQ6.1M distribution functions [34]. This reference set excludes most of the nuclear data used in the PDF global fit, and therefore is not biased by any nuclear corrections.

[^246]:    ${ }^{8}$ As discussed earlier, EPS08/EPS09 also include inclusive $\pi^{0}$ data from the PHENIX experiment at RHIC, with a strong weight in order to better determine the nuclear gluon distribution.
    ${ }^{9}$ Note also that at lower scales the uncertainties of the nPDFs are even more pronounced.
    ${ }^{10}$ The corresponding sets of nPDFs are available upon request from the authors.

[^247]:    ${ }^{11}$ Note that in Mellin moment $N$-space the relation $c^{p / A}(N, Q) / c^{p}(N, Q) \simeq g^{p / A}(N, Q) / g^{p}(N, Q)$ holds approximately for $Q \sim Q_{0}$.

[^248]:    ${ }^{12}$ This back-to-back kinematics matches the LO case and constrains the transverse momentum of the third particle to be zero.

[^249]:    ${ }^{13}$ We have verified that similar results and conclusions are obtained when using either ATLAS or CMS acceptances at central rapidities.

[^250]:    ${ }^{1}$ While bottom squarks ( $\tilde{b}$ ) can be relatively light in some models [33], their contribution to DIS and other relevant cross sections can be neglected, cf. Ref. [23].

[^251]:    ${ }^{2} \mathrm{We}$ use $m_{c}=1.3 \mathrm{GeV}$ and $m_{b}=4.5 \mathrm{GeV}$. The up, down, and strange quark masses $\left\{m_{u}, m_{d}, m_{s}\right\}$ do not play a role in the evolution, as they are less than the initial evolution scale $Q_{0}=$ 1.3 GeV .

[^252]:    ${ }^{3}$ This value, compatible with the current world average, is about $1 \sigma$ below $\alpha_{s}\left(M_{Z}\right)=0.123 \pm 0.004$; hence, the SM fit with this $\alpha_{s}\left(M_{Z}\right)$ value has a higher $\chi_{\text {tot }}^{2}$ (in the last line of the upper table) than a fit with a floating $\alpha_{s}\left(M_{Z}\right)$ (in the last line of the lower table).

[^253]:    ${ }^{4}$ The extent of plausible systematic shifts is determined by matrices of correlated systematic errors, provided by both Tevatron collaborations and implemented in the CT09 [44] and CT10 analyses [25].

[^254]:    ${ }^{1}$ The NNLO contributions produce marginal modifications compared to the NNLL-NLO result included in the CT10 analysis. We examined these contributions by redoing the calculation for $A_{\ell}\left(y_{\ell}\right)$ after adding the exact $\alpha_{s}^{2}$ correction for $W$ bosons produced with non-zero transverse momentum, which captures a large part of the full NNLO effect. The changes were found to be small and inconsequential in the current fit.

[^255]:    *olness@smu.edu
    ${ }^{\dagger}$ soper@uoregon.edu

[^256]:    ${ }^{1}$ Specifically, we use the program of Ref. [1], although there are other programs that can give the same results. The code is available at http://zebu.uoregon.edu/~soper/EKSJets/jet.html

[^257]:    ${ }^{2}$ Specifically, in this figure we use the functions $f_{1}\left(P_{T}\right)=0.1$, $f_{2}\left(P_{T}\right)=0.08 \log \left(P_{T} / M\right)$, and $f_{3}\left(P_{T}\right)=0.06\left\{\left[\log \left(P_{T} / M\right)\right]^{2}-\right.$ $0.1\}$ where $M=150 \mathrm{GeV}$. These curves are for illustrative purposes only, and the $f_{J}\left(P_{T}\right)$ functions differ from the set $f_{J}\left(P_{T}, y\right)$ we will use to parametrize the correlated systematic uncertainties.

[^258]:    ${ }^{3}$ We shall use $\mathcal{E}_{\text {scale }}$ to denote the theoretical systematic error due to scale dependence only, and $\mathcal{E}$ (no subscript) to denote the total theoretical systematic error.

[^259]:    ${ }^{4}$ We scale $P_{T}$ by $M(y)$ to make the argument of the logarithms dimensionless. This quantity provides a simple scaling, and roughly corresponds to scaling by the maximum $P_{T}, P_{T}^{\max } \sim$ $\sqrt{s} /(2 \cosh (y))$, for large $y$.

[^260]:    ${ }^{5} \mathrm{We}$ do not present curves for $y=1$ and $y=2$ because these curves show a rise of the correction as $P_{T}$ decreases from 200 GeV , even though decreasing $P_{T}$ puts us farther from the threshold. This rise is more pronounced for large $y$ than we see for $y=0$ in Fig. 6. We suspect that this behavior is an artifact of kinematic choices in the algorithm for summing threshold logarithms, rather than being a real physical effect.

[^261]:    ${ }^{6}$ Cf., Eq. (5.9) of Dasgupta et al. in Ref. [5]

[^262]:    ${ }^{0}$ This work is based on lectures presented a the CTEQ Summer Schools on QCD Analysis and Phenomenology. http://www.cteq.org
    ${ }^{1}$ See Ref. [4] and also the webpage citation for the 1999 Nobel Prize in Physics at: http://nobelprize.org/
    ${ }^{2}$ Note, for chiral symmetries there are some subtle difficulties that must be handled carefully. In particular, the properties of the parity operator are dependent on the dimensionality of spacetime.

[^263]:    ${ }^{3}$ In Sec. V we will use dimensional analysis to demonstrate that we must introduce an auxiliary length scale $L$ in addition to the regulator $\epsilon$. For other interesting applications of scaling and dimensional analysis $c f$. Refs. [7, [8]

[^264]:    ${ }^{4}$ We will use MKS units here so that our results reduce to the usual undergraduate textbook expressions.

[^265]:    ${ }^{5}$ For simplicity, we will calculate the potential at the mid-point of the wire; the general case is more complicated algebraically, but yields the same result in the $L \rightarrow \infty$ limit.

[^266]:    ${ }^{6}$ Since the factor $\lambda /\left(4 \pi \epsilon_{0}\right)$ has units of potential, the integral must be dimensionless. Also note we have changed the integration limits from $[-\infty,+\infty]$ to $[0,+\infty]$, and the compensating factor of 2 cancels the factor of 2 in $d \Omega_{n} / 2$.

[^267]:    ${ }^{7}$ For an excellent pedagogical analysis of the renormalization group equation $c f$. Ref. [g].

[^268]:    ${ }^{8}$ The reader is invited to verify that the computation of the electric field $\vec{E}(x)$ in a consistent renormalization scheme yields the previous results of Eq. (17).
    ${ }^{9}$ Cf., Ref. 10], Eq. (46) and Eq. (47).

[^269]:    10 Note, for the special case $\mathrm{D}=2$ the potential $V(r)$ has a logarithmic form; see Table II for details.

[^270]:    ${ }^{1}$ The proton beams at IP2 are transversely polarized but due to rapid spin flips they can be spin balanced to get unpolarized protons.

[^271]:    ${ }^{1}$ We note that the measurement of $J / \Psi$ photoproduction at HERA [589, 620 strongly favors an exponential $t$ dependence at $|t|$ below $1 \mathrm{GeV}^{2}$, but the behavior of exclusive hard scattering cross sections at larger $t$ is poorly known. For a conservative error estimate, we do not want to rule out a dipole behavior at $|t|>1 \mathrm{GeV}^{2}$.

[^272]:    ${ }^{2}$ VGG refers to a computer code originally written by M. Vanderhaeghen, P. Guichon, and M. Guidal. To our best knowledge, the code for DVCS presently used by experimentalists employs a model that adopts Radyushkin's DD ansatz 574.

[^273]:    ${ }^{3}$ These energies and luminosities correspond to those given as medium-energy collider design prior to the INT 10-3 program, e.g., $\sqrt{s}=31.0 \mathrm{GeV}$.

[^274]:    ${ }^{4}$ The energies have been chosen to correspond to the preliminary values of the medium and high energy collider designs as given prior to the INT 10-3 program.

[^275]:    ${ }^{1}$ There is a additional term, corresponding to the cubic Casimir; which is parametrically suppressed for large nuclei [772]. This term generates Odderon excitations in the JIMWLK/BK evolution [773, 774].

[^276]:    ${ }^{2}$ Exclusive observables may also be expressed in terms of solutions of the same Yang-Mills equations, but with more complicated boundary conditions than for inclusive observables.

[^277]:    ${ }^{3}$ More precisely, in the QCD case, that asymptotic behavior in rapidity is reached from any initial condition compatible with perturbative QCD in the UV.

[^278]:    ${ }^{4}$ The calculation of $b_{0}, b_{-1 / 6}$ and $b_{-1 / 3}$ has been performed recently in 868 .

[^279]:    ${ }^{5}$ Note that the normalization of the $J / \Psi$ wavefunction in 600 is erroneously reported as a factor of 100 smaller than the correct value; one can readily see this by comparing with the normalization condition defined in 600 a a with the results reported in 823. It is surprising that this error was not noted in 823, in which the results found in [823] are explicitly compared to those in 600 .

[^280]:    ${ }^{6}$ fig. 8 in 885 also shows that the incoherent process quickly dominates the coherent one as a function of $t$, although we note that there was an error in the calculation of the figure and that the curves plotted do not correspond to the equations in the text of the paper.

[^281]:    ${ }^{7}$ We shall take $m_{f}=0.14 \mathrm{GeV}$, the value used when extracting the dipole cross section from $F_{2}$ data.
    ${ }^{8}$ To compare with the HERA data, we take $\epsilon=0.98$.

[^282]:    ${ }^{9}$ Small-x partons do not contribute significantly to the momentum sum rule and a precise matching to the parton distributions at large $x$ and low $Q^{2}$ is lacking.

[^283]:    ${ }^{1}$ Reference 1226 focused on a lower integrated luminosity and a larger cross section.
    ${ }^{2}$ Reference 1226 used only the current $\tau \rightarrow e \gamma$ limit.

[^284]:    ${ }^{3}$ The contribution of the vector leptoquarks is less clear, for reasons explored in 1226, so we restrict our discussion to the scalar LQs.

[^285]:    ${ }^{4}$ We limit our discussion here to the scenario of "minimal field content" described in 1236 .

[^286]:    ${ }^{5}$ The Bjorken scattering variable is given by $y=Q^{2} / s_{e p} x=1 / 2(1-\cos \hat{\theta})$ where $\hat{\theta}$ is the decay polar angle of the lepton relative to the incident proton in the center-of-mass frame.

[^287]:    ${ }^{6}$ See section 6.3 .2 for a description of the notation. This leptoquark's interactions are given by the Lagrangian terms $\lambda \bar{d}_{R} \ell_{L} \tilde{S}_{1 / 2}^{L}+$ h.c. Also note that this leptoquark evades limits from $\tau \rightarrow e \gamma$ as explained in section 6.3.2

[^288]:    ${ }^{1}$ There is no accelerator problem with using lower energy electron beams.. According to statements from EIC physicists, using electron energies below 5 GeV would not contribute significantly to the physics goals.

[^289]:    ${ }^{2}$ http://conferences.jlab.org/eic2010

[^290]:    ${ }^{1}$ Specifically, there were 1333 DIS data points used out of the 1925 total. 84

[^291]:    ${ }^{2}$ The CCFR arrangement used two C-shaped sections with a horizontal crack at the center to allow placement of hall probes for field calibration. This crack would be eliminated in NuSOnG and instead small slots could be included for this purpose.

[^292]:    ${ }^{\text {a }}$ This "internally self-consistent analysis technique" ${ }^{2}$ was employed by the NuTeV experiment. For NuTeV, however, the statistics were limited and some external data were also used as input.

[^293]:    ${ }^{\mathrm{b}}$ For a recent review of nuclear shadowing see, e.g. Ref. 23.

[^294]:    ${ }^{\text {c }}$ The proposal for the MINER $\nu \mathrm{A}$ experiment is presented in Ref. 32, and the experiment webpage is located at: http://minerva.fnal.gov/.

[^295]:    ${ }^{\mathrm{d}}$ If we work at NLO, $f_{c}\left(x, \mu=m_{c}\right)$ should be strictly greater than or equal to zero; at NNLO and beyond the boundary conditions yield a negative PDF of order $\sim \alpha_{s}^{2}$.

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[^301]:    1 This point has frequently been overlooked in lattice QCD calculations.

[^302]:    ${ }^{2}$ This would now amount to 2.9 MeV given that the average experimental width of the $\eta_{c}$ has increased to 30 MeV [7].

[^303]:    ${ }^{3}$ This method is often called 'nonperturbative' in the lattice QCD literature.

[^304]:    ${ }^{4}$ For a meson containing an NRQCD quark the energy obtained from the 2-point and 3-point fits is not its mass. However that is irrelevant here since it cancels.

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[^306]:    ${ }^{1}$ In 35 these are called $\chi_{\text {conn }}$ and $\chi_{d i s c}$.

[^307]:    ${ }^{2}$ We are ignoring nonperturbative short-distance physics (for example, small instantons) which can contribute to coefficient functions but is typically nonleading.

[^308]:    ${ }^{3}$ If this isn't the case, then coefficient function $h$ will not equal one, but rather will be a series in $\alpha_{\overline{\mathrm{MS}}}$.

