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1 Executive Summary

This is the final report on grant DE-FG05-96ER40979 from the U.S. Department of Energy supporting the research of the Theoretical High Energy Physics group at the Supercomputer Computations Research Institute (SCRI) at Florida State University. The research primarily involved lattice field theory simulations such as Quantum Chromodynamics (QCD).

Although QCD is generally accepted as the theory which describes the strong interactions responsible for nuclear binding, convincing computations of the properties of the elementary particles from first principles are still elusive. The problem lies in the fact that for data at the "low" energies involved (~ 1 GeV), the coupling constant in QCD is large, preventing application of the physicist's usual tool, perturbation theory. Non-perturbative computations are necessary and they appear possible only via large scale numerical simulations. Especially simulations of "full QCD", including the effect of light dynamical quarks, are extremely CPU time consuming. The scientists in SCRI's lattice gauge theory group have been in the forefront of such numerical simulations since the inception of SCRI in 1985.

SCRI scientists have developed highly efficient algorithms and codes, which are fairly easily portable to various supercomputers, as well as workstations (used mainly for code development). In some cases the most frequently used code segments have been hand optimized for a particular computer architecture. With these codes they have performed numerical simulations of many interesting physics problems. Most of these computations were carried out on the CM-2 and the 50 Gigaflap QCDSF machine at SCRI. Other, smaller, calculations were carried out on the workstation cluster at SCRI, while most of the computing done with the MILC collaboration used resources at national supercomputer centers.

Among the works completed by the members of the lattice group and their outside collaborators in QCD simulations are extensive hadronic spectrum computations with both Wilson and staggered fermions. Heavy-light meson decay constants were another focus of research, in particular concerning differences between quenched and dynamical calculations. Studies of the finite temperature behavior of QCD have also been a major activity within the group.

A major research topic was the study of improved lattice actions, designed to diminish finite lattice spacing effects and thus accelerate the approach to the continuum limit. Most of this work was carried out in the quenched approximation. Very encouraging results were obtained.

In the second half of the funding period, a major focus of the group has been the use of a new lattice fermion representation, Overlap fermions, that has achieved the much desired goal of preserving the chiral symmetry properties of the continuum theory at finite lattice spacing. After developing an algorithm for the numerical simulations of overlap fermions, the SCRI group has completed the first studies of the relation between chiral symmetry breaking and topology using this new formalism.

2 Quantum Chromodynamics

2.1 Dynamical simulations with “standard” fermions

2.1.1 Zero-temperature simulations and spectroscopy

Bitar, Edwards, Heller, and Kennedy continued QCD simulations on the CM-2, using dynamical Wilson fermions with $\kappa = 0.1596, 0.1600$ and 0.1604 , at gauge coupling $\beta = 5.5$ on $16^3 \times 32$ lattices. Measurements were made of the hadronic spectrum, and of axial and vector current matrix elements, and the heavy quark potential. The lattice spacings were determined to be about 0.1 fm, comparable to those of earlier simulations with two flavors of dynamical staggered fermions done under the aegis of the HEMCGC collaboration. The pion masses obtained at $\beta = 5.5$ are $m_\pi a \approx 0.38, 0.33$, and 0.27 . These small pion masses confirm the findings from the previous simulations at $\beta = 5.3$ that chiral symmetry can be restored for Wilson fermions in the continuum limit [1].

As a member of the “MIMD Lattice Calculation” (MILC) collaboration, Heller was involved in a study of two-flavor QCD with staggered fermions. Ensembles of gauge field configurations were generated at several different gauge couplings, *i.e.* lattice spacings, and several different quark masses down to about half the strange quark mass. Spectroscopy calculations on these ensembles were used for a first continuum extrapolation of staggered spectroscopy in full two-flavor QCD [2].

2.1.2 QCD thermodynamics

Heller and Kennedy were members of another large collaboration that studied the phase transition/crossover from the hadronic phase at low temperatures to the quark-gluon plasma phase at high temperature for two flavors of staggered fermions on lattices with temporal extent $N_t = 8$, pushing this study closer to the continuum limit. These calculations were done on the CM-2 at the Pittsburgh Supercomputer Center. The crossover and some properties of the high temperature phase have been studied for quarks with rather light mass, $m/T = 0.05$, to study the behavior as the massless limit is approached [3].

Heller, as a member of the MILC collaboration, was involved with several other studies of the finite temperature behavior of QCD with staggered fermions. This included thermodynamics on an $N_t = 12$ lattice [4], further pushing towards the continuum limit, the determination of the equation of state on $N_t = 6$ lattices [5] and the investigation of which chiral symmetry is restored at high temperature [6].

2.1.3 Parity-flavor breaking phase

Bitar has completed a study of the possible existence in QCD with two flavors of Wilson fermions of a parity-flavor breaking phase at values of $\kappa > \kappa_c$. This was done by numerical simulations on volumes of L^4 with $L = 6, 8, 10$ of a QCD modified by an explicit parity-flavor breaking term. Finite size analysis and extrapolation in the size of the explicit breaking term all lead to the conclusion that (a) such a a parity-flavor

breaking phase exists in the strong coupling region, but that (b) such a phase is not likely to exist for larger values of β relevant to the continuum limit, in contrast to earlier assertions [7].

Parity and flavor symmetry is not broken in massive continuum QCD; hence, a non-zero condensate for an operator that breaks parity and flavor symmetry indicates massless quarks. Using this fact, Bitar, Heller and Narayanan made a proposal to measure the chiral condensate in lattice QCD using Wilson fermions with an operator that breaks parity and flavor in addition to chiral symmetry [8]. This operator has the advantage that it is only non-zero if the fermion is massless and chiral symmetry is spontaneously broken. As such there is no additive renormalization in contrast to the usual operator $\bar{\psi}\psi$. Furthermore, one can get a good estimate of the chiral condensate using this method by evaluating a few low lying eigenvalues of the hermitian Wilson Dirac operator, $H(m) = \gamma_5 W(-m)$, where $W(m)$ is the usual Wilson-Dirac operator with mass m .

2.1.4 Multi-flavor QCD

Perturbation theory predicts that the β -function for QCD with 16 flavors has a second zero at some $g^{*2} \approx 0.5$, besides the one at $g^2 = 0$. For couplings larger than g^{*2} the β -function should therefore have the opposite sign than for QCD with few flavors. Some indications, that this scenario remains valid beyond perturbation theory, were found in numerical simulations with staggered fermions in [9]. Heller used the Schrödinger functional, extended to staggered fermions, to directly compute a running coupling, with the scale given by the size of the system simulated. His results, [10], unambiguously confirm the previous findings.

2.2 Dynamical simulations with clover fermions

2.2.1 Zero-temperature simulations and spectroscopy

The ultimate goal of the $\mathcal{O}(a)$ improvement program is to improve simulations of dynamical fermions. Over the years the SCRI lattice group has gained considerable experience in simulations with dynamical Wilson fermions. In that tradition an investigation of the hadron spectrum using two dynamical quark flavors of improved Wilson (*i.e.*, *Sheikholeslami-Wohlert* or *clover*) fermions with the improvement coefficient, c_{sw} , as determined non-perturbatively by the ALPHA collaboration [11] was initiated. Simulations are underway at $\beta = 6/g^2 = 5.2$ of the standard Wilson gauge action, the strongest coupling for which c_{sw} has been determined. Preliminary results indicate that this corresponds to a lattice spacing of about 0.14 fm. The simulations are done on a $16^3 \times 32$ lattice, with some additional runs on $8^3 \times 16$ and $12^3 \times 24$ lattices for various checks. According to previous experience, physical volumes of about 2.0 fm are required in order to avoid significant finite size effects. Thus a $16^3 \times 32$ lattice should be sufficient at this coupling. The first simulation with 1000 trajectories, after thermalization, at $\kappa = 0.1340$ gives $m_\pi = 0.631(2)$ on the $16^3 \times 32$ lattice and $m_\pi/m_\rho = 0.801(4)$. A second run at $\kappa = 0.1350$ with so far 2000 trajectories

gives $m_\pi = 0.414(2)$ with $m_\pi/m_\rho = 0.703(6)$. At least 3 different values for the quark mass will be used on the large volume in order to make reliable extrapolations in the quark mass. This is necessary since simulations at the physical values of the light up and down quark masses cannot be afforded at present. Based on experience with quenched simulations, we expect about 5% scaling violations of physical observables with respect to their continuum values.

2.2.2 QCD thermodynamics

Heller, with the MILC collaboration, completed an investigation of the finite temperature deconfinement transition/crossover with $\mathcal{O}(a)$ improved dynamical Wilson quarks, the so-called clover fermions, and an improved gauge action introduced by Lüscher and Weisz. The clover coefficient was set to the tadpole improved tree-level value since for this action combination non-perturbative values have not been determined. Use of the improved fermions eliminated the strange finite temperature behavior, believed to be due to lattice artifacts, that has been observed with Wilson quarks on finite temperature lattices with $N_t = 4$ and 6. However, comparing with results using staggered quarks there appear to still be large scaling violations present at the large couplings used [12].

Edwards and Heller also have carried out simulations to determine the behavior of non-perturbatively $\mathcal{O}(a)$ improved clover fermions with standard Wilson gauge action at finite temperature on lattices with small temporal extent, $N_t = 4$ and 6, where earlier simulations with unimproved Wilson fermions have shown strange, unexpected behavior (e.g., first order phase transition signals at intermediate quark mass) that is generally attributed to lattice artifacts. The results are somewhat discouraging in the sense that at the couplings for which the clover coefficient has been determined non-perturbatively, the finite temperature crossover occurs at such large pion masses as to be physically uninteresting. On lattices with temporal extent $N_t = 4$ and 6, one would have to know the clover coefficients for stronger coupling to have any chance to see light quark physics in the finite temperature crossover region. On the positive side, the crossover turned out much smoother than on comparable systems with unimproved Wilson fermions [13].

2.3 Quenched spectroscopy

Heller, as a member of the MILC collaboration, was involved in a systematic investigation of quenched spectroscopy with staggered fermions [14]. Particular emphasis was put on controlling the chiral extrapolation from the masses used in the simulations, namely quark masses only down to about half the strange quark mass, to the actual quark masses of the light quarks. Quenched chiral perturbation theory was used to guide the extrapolation.

A striking prediction of QCD going beyond the naive quark model is the existence of so-called hybrid mesons, where the quark and anti-quark are in a color octet state and gluons are present to make the entire object a color singlet. The MILC collaboration has done studies of the masses of such hybrid mesons in the quenched approximation,

both with Wilson and clover quarks, with quark masses around the strange and the charm quark mass [15].

2.4 Heavy-light quark physics

With former SCRI postdocs Collins (Glasgow) and Sloan (Kentucky), and with Davies and Ali Khan (Glasgow) and Shigemitsu (Ohio State), Heller used NRQCD to study mesons containing one heavy and one light quark. These simulations used the old HEMCGC configurations with two-flavors of dynamical staggered quarks. Wilson, and later clover improved fermions were used for the light quark. The study concentrated on the spectroscopy of B mesons, including radially excited and P -wave states, and the decay constant f_B [16, 17, 18]. Particular emphasis was put on examining the dependence on the heavy quark mass in an effort to check predictions, and determine parameters, of the "Heavy Quark Effective Theory." Their results for the B spectrum are the most extensive of any lattice calculation, while their results of the mesonic decay constants f_B and f_{B^*} agree well with those that use a different treatment of the heavy quark.

Heller, as a member of the MILC collaboration, was also involved with a systematic study of heavy-light decay constants using Wilson quarks for both light and heavy quark, but with the heavy quark interpreted according to the Fermilab approach. In addition, static-light calculations were used to anchor the fits as function of the heavy quark mass. Particular emphasis was put on chiral and continuum extrapolations with controlled systematic errors, including an estimate of the error from using the quenched approximation [19].

2.5 Studies of improved actions

The ultimate goal of numerical simulations is to understand the continuum behavior of QCD, to verify that it correctly describes nature, and to help experiments determine Standard Model parameters by computing the necessary hadronic matrix elements. One is, of course, forced to work on finite lattices and hence the simulation results suffer from discretization errors and finite physical volume errors.

Most QCD simulations with Wilson fermions carried out before about 1993 have used the standard Wilson gauge and fermionic action. However, the Wilson gluonic action has finite- a errors of $\mathcal{O}(a^2)$ and the fermionic action has $\mathcal{O}(a)$ errors. A brute force reduction of these discretization errors would be prohibitively expensive. An alternative approach is the Symanzik improvement program. Terms that are irrelevant in the continuum limit are added to the action to eliminate the discretization errors order by order in the lattice spacing. For example, adding 6-link operators to the Wilson gauge action eliminates the $\mathcal{O}(a^2)$ discretization errors. The remaining errors are $\mathcal{O}(a^4)$. Similarly, adding a $\sigma \cdot F$ term to the Wilson fermionic action eliminates $\mathcal{O}(a)$ errors. This is the Sheikholeslami-Wohlert or "clover" fermion action. The procedure can be extended to higher orders in the lattice spacing.

The SCRI lattice group has embarked on a systematic study of improvements in the fermionic and gluonic actions. The goal was to test these improvements in a

full QCD simulation. The steps have involved (1) comparing Wilson and “tadpole” clover improved fermions on a previously generated gauge ensemble with two flavors of staggered fermions. (2) measuring Wilson and “tadpole” clover spectroscopy on $\mathcal{O}(a^2)$ improved quenched gauge fields. (3) studying higher order “tadpole” improved fermionic spectroscopy on improved quenched gauge fields, and (4) determining and testing a non-perturbatively improved clover fermion action.

2.5.1 Tadpole improved clover fermions

Edwards and Heller, with former SCRI postdocs Collins (Glasgow) and Sloan (Kentucky) carried out the comparison of spectroscopy with Wilson and clover fermions, with the tadpole improved tree-level value for the clover coefficient, on a lattice with inverse spacing of 2 GeV, the ensemble created at SCRI by the HEMCGC collaboration with two flavors of dynamical staggered quarks. They showed that a higher order chiral perturbation theory ansatz works well to extrapolate their mass results towards the chiral limit. They found that the largest effect of the clover term is an additive shift in the vector mass. Since this vector mass is used to determine the physical quark mass, this shift feeds into all spectroscopy predictions. While the mass predictions with Wilson fermions deviate from the experimentally known masses by discretization errors of about 20%, the improved clover fermions lead to discretization errors of only a few percent [20].

The same researchers carried out the second step, producing one of the most accurate continuum extrapolations of the (quenched) light hadron spectrum to date. An $\mathcal{O}(a^2)$ and tadpole improved (to 1-loop) gauge action was used, with the gauge coupling chosen to cover lattice spacings in the range 0.16 fm to 0.42 fm. Simulations were performed with both the Wilson and the tadpole improved clover quark actions. Large lattices of extent $16^3 \times 32$ were used to avoid the problem of exceptional configurations. Dimensionless ratios of hadron masses to the string tension were computed. Their results [21] indicate 20% scaling violations for clover and 50% for Wilson fermions over the range of lattice spacings considered. Chiral extrapolations were made of quark masses to the physical ρ/π ratio, and interpolations to masses in the strange quark regime. The latter results provided a very accurate determination of the scaling form showing a 94% confidence level for the clover action using the expected $\mathcal{O}(a^2)$ form and 3% to the form $\mathcal{O}(a)$. The Wilson action which is expected to scale like $\mathcal{O}(a)$ shows a significant sub-leading correction of $\mathcal{O}(a^2)$ over the region of interest. The conclusion is that the clover action provides a more accurate and reliable estimate of the continuum fermionic action than the Wilson action.

Klassen has carried out the third step, in collaboration with Lepage (Cornell) and Alford (IAS, Princeton). The goal of this work was to reduce the fermionic discretization errors down to the same order as the gluonic errors, $\mathcal{O}(a^4)$. As a first step in this direction they [22] presented the “D234” light quark action, which has only $\mathcal{O}(a^3)$ scaling violations. This action showed many promising features, in particular, greatly improved dispersion relations for the mesons. However, the scaling violations in other parts of the hadron spectrum were still somewhat too big on very coarse lattices (roughly 20% at 0.4 fm).

2.5.2 Non-perturbative $\mathcal{O}(a)$ improvement

Using the tadpole value of the clover coefficient reduces the leading discretization errors from $\mathcal{O}(a)$ only to $\mathcal{O}(\alpha^n a)$ with $n = 1$ or 2 if using the tree-level or one-loop coefficient respectively. Even if the coefficient of this leading correction is small, it should be included, giving an additional free parameter for the continuum extrapolation and therefore increased errors.

Using a newly developed finite size technology based on the Schrödinger functional, the ALPHA collaboration (of which Sint is a member) has recently [23, 24] been able to determine some of the coefficients that arise at $\mathcal{O}(a)$ improvement non-perturbatively, using numerical simulations. With the improvement coefficients determined in this way, one may expect a complete elimination of $\mathcal{O}(a)$ errors in spectral and on-shell quantities. In particular this means that the required continuum extrapolations should be easier, since one may directly use an ansatz with a leading quadratic dependence on a .

After full $\mathcal{O}(a)$ improvement has been implemented the violations of chiral symmetry appear to be strongly reduced. In particular, the chiral symmetry “point” (the critical κ) is then defined to sufficient accuracy, its inherent ambiguity being reduced by one order in the lattice spacing. By imposing naive chiral Ward identities as normalization conditions, the ALPHA collaboration then proceeded to fix the non-singlet axial and vector current normalization constants. The precision achieved was better than 1 percent, which will strongly reduce the corresponding uncertainty of the pion decay constant (previously of the order of 10 percent) in future simulations [25].

Even with the above mentioned new technique some of the improvement coefficients remain elusive and one may have to rely on perturbative estimates. Therefore S. Sint and P. Weisz (MPI, Munich) have computed a number of improvement coefficients to one-loop order of perturbation theory. Their method also allowed to evaluate the complete cutoff effects in correlation functions at the tree and at the one-loop level [25]. This in turn can be used as a guide when parameters are to be chosen for the non-perturbative investigations.

Edwards, Heller and Klassen have extended the non-perturbative $\mathcal{O}(a)$ improvement of the Wilson quark action to coarser lattices. This was possible, since they found that the quark mass dependence of the non-perturbative clover coefficient is very weak. They could do the simulation at non-zero quark mass, avoiding problems with near zero modes on coarse lattices, and extend the $\mathcal{O}(a)$ improvement to lattices as coarse as $a = 0.17$ fm or $\beta \geq 5.7$ for the Wilson gauge action [26, 27].

To test the improvement, Edwards, Heller and Klassen also did spectroscopy calculations on these coarse lattices. The large range of lattice spacings obtained by combining the new results with earlier ones on finer lattices, together with the accurate string tension measurements recently performed (cf. section 3), [28], allow the first convincing demonstration of the efficiency of non-perturbative $\mathcal{O}(a)$ improvement [27]. They found that scaling violations of hadron masses on the coarsest lattice drop from 30 – 40% for the standard Wilson action to only 2 – 3% for the improved one.

Edwards, Heller and Klassen also determined the clover coefficient non-perturba-

tively in the background of gauge fields generated with the Lüscher-Weisz 1-loop improved gauge action [26]. In this case, lattices as coarse as $a = 0.25$ fm could be reached.

2.5.3 Anisotropic lattices and $\mathcal{O}(a)$ improvement

Klassen and his collaborators have shown that part of the still rather big scaling violations of the highly improved D234 fermion action are due to “ghost branches” (whose origin are the higher order terms in the improved action) in the energy-momentum dispersion relation. The ghost branches can be pushed up in energy by going to an anisotropic lattice, whose lattice spacing in the “time” direction is smaller than the spatial ones [29]. Anisotropic lattices have been investigated in the past, but without tadpole improvement there are large violations of $O(4)$ symmetry, even in on-shell quantities. With Symanzik- and tadpole-improved glue, however, these errors stay at the 2–3% level, making improved glue on anisotropic lattices as easy to use, and as accurate, as on isotropic lattices.

Anisotropic lattices, where the temporal lattice spacing is smaller than the spatial one, have numerous advantages in studies of lattice thermodynamics, heavy quarks, and particles with bad signal to noise properties, like glueballs and P-state mesons.

The groundwork for the use of improved quark actions on anisotropic lattices was laid by Klassen *et al.* in [30], where a very simple and general method of constructing classically improved lattice quark actions was described. One of the actions discussed in detail there is the D234 action, which classically has only $\mathcal{O}(a^3)$ errors. Simulation results for the hadron spectrum of the tadpole improved D234 action on anisotropic lattices were presented [29]. Most quantities, especially those related to violations of rotational symmetry, showed much more continuum-like behavior on coarse lattices than all other known quark actions. However, other quantities were not significantly better than when calculated with less improved actions, like the tadpole improved clover action.

This was explained in [31] as being due to residual $\mathcal{O}(a)$ violations of chiral symmetry at the quantum level (which are, in a sense, “orthogonal” to the $\mathcal{O}(a^2)$ violations of rotational symmetry that were largely eliminated in the D234 action). It was argued in [31] that one should use Schrödinger functional techniques (cf. subsec. 2.5.2) to eliminate these errors for quark actions on improved glue. This should finally yield quark actions that give accurate results (on the few percent level) for *all* quantities on coarse lattices.

2.5.4 Improved staggered fermions

Staggered, or Kogut-Susskind fermions preserve a remnant chiral symmetry at finite lattice spacing and so naturally have scaling violations of order $\mathcal{O}(a^2)$ only. However, flavor symmetry is broken at finite lattice spacing, and quite strongly so at presently tractable lattice spacings. The flavor symmetry breaking is mediated by exchange of gluons with momenta at the corners of the Brillouin zone. By adding 3-, 5- and 7-link gauge field staples to the nearest neighbor hopping term, coupling to such gluons can

be suppressed and flavor symmetry breaking reduced. Adding, in addition, a straight 3-link hopping term, all scaling violations of order $\mathcal{O}(a^2)$ can be eliminated at the classical (tree) level. Heller, with the MILC collaboration, has investigated the scaling behavior of such improved staggered fermions in the quenched approximation. They found that both meson and nucleon masses show very little scaling violations [32]. Encouraged by these results, the MILC collaboration has started dynamical simulations with these improved staggered fermions.

2.6 Spectral flow and topology

Chiral symmetry plays an important role in QCD. It has been conjectured that gauge field topology is important in understanding spontaneous chiral symmetry breaking. However, the determination of the relation of topology with chiral symmetry on the lattice has been plagued with many problems. The spectrum of the hermitian Wilson-Dirac operator $H_w(m) = \gamma_5 D_w(-m)$, where $D_w(m)$ is the usual Wilson-Dirac operator with mass m , carries information about gauge field topology [33] and also about the spontaneous breakdown of chiral symmetry [8].

Zero crossings of the eigenvalues of $H_w(m)$ are due to the topological content of the gauge field background. Edwards, Heller and Narayanan carried out a comprehensive study of the spectral flow of $H_w(m)$, with and without a clover term, on a variety of SU(2) and SU(3) lattice gauge field ensembles [34, 35]. The spectral flow method involves slowly increasing the mass and observing the eigenvalue spectrum. The net number of zero crossings — down minus up — up to mass m gives the topological charge. Ensembles generated from the Wilson gauge action, an improved gauge action, and several two-flavor dynamical quark ensembles were considered. It was found that the spectrum could be characterized by two regions divided by m_1 — the location of the first level crossing zero. For $m < m_1$, corresponding to positive physical quark mass, the spectrum has a gap. In region II, $m_1 < m \leq 2$, no spectral gap was found. The absence of a spectral gap implies that the density of zero eigenvalues, $\rho(0; m)$, could be non-zero for $m_1 < m \leq 2$. Indeed it was shown that $\rho(0; m)$ for the Wilson gauge and fermion action is non-zero, but decreases exponentially in the inverse lattice spacing and becomes only zero in the continuum limit [35]. This result shows that the approach to the continuum limit for the quenched hermitian Wilson-Dirac operator is not at all the same for the positive physical quark mass and the unphysical quark mass side of the critical region m_1 . Also, a non-zero $\rho(0; m)$ has adverse implications for the efficiency of practical implementations of the overlap Dirac operator and for the L_s dependence of domain wall fermions [36].

Another result of the study of the levels crossing zero in the region $m_1 < m \leq 2$ was the determination of the topological susceptibility and the size distribution of zero modes. The eigenvalues crossing through zero that occur in the large mass region correspond to localized eigenmodes and the localization size decreases monotonically with the crossing point down to a size of about one lattice spacing. These small modes are unphysical and do not affect the topological susceptibility. The results for the topological susceptibility are in agreement with those obtained by other groups using different methods.

The size distribution was studied for various β in $SU(2)$ and $SU(3)$ gauge theory. When excluding the contribution for the small modes that do not affect the topology, broad peaks for the size distribution are seen around 5 lattice units in a volume of 16^4 sites, independent of the gauge coupling and thus not at constant physical size [34, 35]. This does not agree with predictions for the instanton size distribution, for which a peak at a size of about 0.4 fm is expected.

Edwards, Heller and Narayanan also computed the chiral condensate in four-dimensional non-Abelian gauge theories with Majorana fermions in the adjoint representation. Gluinos are expected to condense in supersymmetric Yang-Mills theories even in finite volume. Instantons cannot explain a bilinear condensate of gluinos since the number of zero modes in a single instanton $SU(N)$ background gauge field is equal to $2N$. However, one could have truly quantum backgrounds that result in a bilinear condensate of gluinos and as such cannot be seen in any semi-classical approximation. By studying the spectral flow of $H_w(m)$ in $SU(2)$ gauge field backgrounds with the fermion in the adjoint representation, they showed that there were a significant number of configurations with only doubly degenerate levels crossing zero. The fraction of configurations with these half integer topological charges appeared to remain constant as the lattice spacing was decreased by a factor of two. This result indicates that, at least for the couplings studied, the presence of fractional topological charge configurations is not just a lattice artifact [37].

2.7 Overlap fermions

Since the beginning of lattice gauge theory, the regularization of chiral fermions has been a severe problem. When regulating fermions on a lattice, typically, unwanted doublers with opposite chirality appear. These doublers can be lifted (given mass of the order of the cut-off) at the cost of explicitly breaking chiral symmetry. These are the Wilson fermions. Alternatively, a remnant of chiral symmetry can be retained, with a smaller number of additional "flavors." These are the staggered fermions, with the drawback that they come in multiples of four flavors with the flavor and full chiral symmetry broken at finite lattice spacings. Additionally, staggered fermions do not have exact zero modes in topologically non-trivial gauge field backgrounds obscuring studies of the relation between topology and spontaneous chiral symmetry breaking in QCD.

Recently, significant progress has been made in overcoming the problems of regularizing chiral gauge theories using the overlap formalism [33]. In particular the study of vector gauge theories (where one does not need to worry about anomalies) with massless fermions became possible. Based on the overlap formalism, Neuberger proposed a particularly simple form for the fermion determinant and the fermion propagator [38]. Including a fermion mass μ , Neuberger's overlap Dirac operator is given by

$$D(\mu) = \frac{1}{2} [1 + \mu + (1 - \mu)\gamma_5 \epsilon(H_w(m))] \quad (2.1)$$

with $H_w(m) = \gamma_5 D_w(-m)$. Here $D_w(m)$ is the usual Wilson-Dirac operator, and $\epsilon(H_w(m)) = H_w(m)/\sqrt{H_w^2(m)}$. The Wilson-Dirac mass m has to be chosen in the

supercritical regime, $m_c < m < 2$, where $-m_c$ is the critical mass of standard Wilson fermion spectroscopy.

Edwards, Heller and Narayanan have developed methods to deal with $\epsilon(H_w(m))$, as described in Section 4. They used the optimal rational approximation to $\epsilon(H_w(m))$ for a study of chiral symmetry in quenched QCD [39]. Overlap fermions have exact zero modes in topologically non-trivial gauge field backgrounds. Disentangling contributions from these exact zero modes simplified the numerical computations and allowed to compute the condensate and chiral susceptibilities for a wide range of fermion masses, including the massless limit.

The Goldstone pions, associated with the spontaneous breaking of chiral symmetry dominate the low-energy, finite-volume scaling behavior of the Dirac operator spectrum in the microscopic regime, defined by $1/\Lambda_{QCD} \ll L \ll 1/m_\pi$, with L the linear extent of the system. The properties in this regime are universal and can be characterized by chiral random matrix theory (RMT) within three ensembles, depending on symmetry properties of the Dirac operator and the sector of fixed topology (entering via the number of exact zero modes). The overlap Dirac operator has the same chiral properties as the Dirac operator in the continuum, and it has exact zero modes in topologically non-trivial gauge fields. It is thus well suited to test the predictions of RMT. Edwards, Heller, Kiskis (UC Davis), and Narayanan computed the low lying eigenvalues of the massless overlap Dirac operator for examples in all three universality classes – SU(2) in the fundamental representation for the orthogonal ensemble, SU(3) in the fundamental representation for the unitary ensemble and SU(2) in the adjoint representation for the symplectic case – and in the sectors with zero or one exact zero modes. The distributions of the lowest (non-zero) eigenvalue was compared to the predictions of chiral RMT. Excellent agreement was found [40].

Edwards, Heller, Kiskis and Narayanan extended the study of small eigenvalues of the overlap Dirac operator to quenched gauge theories in the high-temperature, deconfined phase. They found exact zero modes indicating that gauge field configurations with non-trivial topology persist in the high temperature phase. They also found that the spectrum of the non-zero eigenvalues has two parts separated by a region in eigenvalue where the density is essentially zero. The distribution of very small non-zero eigenvalues of the overlap Dirac operator is well-described by a dilute gas of non-interacting instantons and anti-instantons and suggests the existence of a chiral condensate which was confirmed with a direct stochastic estimate [41].

2.8 Staggered Dirac spectra and random matrix theory

As mentioned, the low eigenvalues of the Dirac operator in the microscopic regime, $1/\Lambda_{QCD} \ll L \ll 1/m_\pi$, are predicted to be universal within three classes, chiral orthogonal, chiral unitary and chiral symplectic, depending only on symmetry properties of the Dirac operator. Heller, together with Damgaard (Niels Bohr Institute) and Krasnitz (Algarve, Portugal) verified numerically the chiral unitary case with staggered fermions in the fundamental representation of SU(3) [42] and Edwards, Heller and Narayanan verified the chiral orthogonal case with staggered fermions in the adjoint representation of SU(2) and SU(3) [43]. Contrary to overlap fermions,

ered fermions do not seem to “feel” effects of topology on the ensembles at
 ently accessible gauge couplings [44], and thus staggered fermions only probe the
 dictions of RMT in the topologically trivial sector.

2.9 Finite Size Scaling of the Chiral Condensate

In the rather extreme regime $V \ll 1/m_\pi^4$, the QCD partition function depends on the
 fermion mass only in the combination $\mu \equiv V\Sigma m$, where Σ is the chiral condensate.
 In this regime precise finite-volume scaling functions apply which can be computed
 analytically in random matrix theory. Damgaard, Edwards, Heller and Narayanan
 confronted these predictions with data from quenched lattice gauge theory simula-
 tions. Using staggered fermions in both the fundamental and adjoint representations,
 and gauge groups $SU(2)$ and $SU(3)$, they were able to test simultaneously all of the
 three chiral universality classes. With overlap fermions they also tested the predic-
 tions for gauge field sectors of non-zero topological charge. Agreement was found in
 most cases [45] and the origin of the deviations were understood.

3 Pure Gauge Theory

Heller, together with Karsch (Bielefeld) and Rank, a graduate student from Biele-
 feld who visited SCRI from July 96 to June 97, continued the study of the high
 temperature phase of pure glue $SU(2)$ gauge theory. They concentrated on an ef-
 fort to compute the electric and magnetic gluon screening masses and to inves-
 tigate their dependence on the temperature. For this they computed the gluon
 propagator on gauge configurations fixed to Landau gauge for a temperature range
 $1.3 \lesssim T/T_c \lesssim 10^4$. With this large temperature range they could verify the expected
 behavior $m_m(T)/T \propto g^2(T)$ for the magnetic screening mass, and $m_e(T)/T = cg(T)$
 for the electric one, with $g(T)$ a running coupling that depends logarithmically on
 the temperature. The constant c , however, turned out more than two times larger
 than the perturbative prediction. To test scaling, and improve rotational invariance,
 they extended their computations to a tree-level Symanzik improved action [46].

Extrapolation of spectroscopic results to the continuum limit require an accurate
 determination of the scale. Edwards, Heller and Klassen have revisited the deter-
 mination of the string tension from the potential in pure $SU(3)$ gauge theory using
 the Wilson gauge action. Using previous world data and new high statistics mea-
 surements on coarse lattices, an improved analysis procedure has allowed them to
 determine the string tension and another short distance scale, r_0 , called the Sommer
 scale. The new procedure has allowed determination of these scales to about 1% ac-
 curacy [28]. Another result emerging from this study was an accurate determination
 of the Λ -parameter of quenched QCD, $\Lambda_{\overline{MS}} = 247(16)$ MeV.

The study of heavy systems, such as glueballs, hybrids and heavy quarkonia is
 difficult for two reasons: (i) since the masses or energies involved are large, in lattice
 units, lattice effects are large; (ii) the correlation functions decrease rapidly into sta-
 tistical noise making a reliable extraction of the masses problematic. Both of these

problems can be avoided by using anisotropic lattices with the lattice spacing in the temporal direction smaller than in the spatial directions. However, a precise knowledge of the renormalized anisotropy is necessary, and a precise scale determination is needed. The non-perturbative relation between bare anisotropy, bare coupling and renormalized anisotropy was recently determined by Klassen [47]. Edwards, Heller and Klassen have made a determination of the lattice scale for several renormalized anisotropies as function of the bare coupling. Heller has also generalized the perturbative computation of Wilson loops that he did with Karsch in 1985 [48] to the case of anisotropic lattices. This will help in defining "improved lattice couplings" on the anisotropic lattices.

4 Algorithm Development

Edwards, Horváth, and Kennedy have studied how instabilities arise and how reversibility fails in molecular dynamics (MD) trajectories used in the HMC algorithm [49]. They showed that there are two kinds of instabilities; those due to too large a step size for the discretization of the equations of motion, and those due to the intrinsic chaotic nature of the classical trajectories themselves. They showed that the classical equations have a Liapunov exponent describing a sensitivity to round-off errors in the integration. This Liapunov exponent times the correlation length is roughly constant in the scaling region of pure gauge and full QCD indicating that chaotic reversibility errors should not be a significant problem even in the continuum limit. They conclude that 32-bit floating point precision is sufficient for computations which are feasible in the near future.

Horváth and Kennedy have completed a detailed free-field theory analysis of the behavior of local Hybrid Monte Carlo (overrelaxation) algorithms for local actions. Their conclusions differ from previous expectations in that they showed that if the local lattice site updates are done in a suitable (lexicographical) order it is possible to eliminate critical slowing down entirely ($z = 0$) for the integrated autocorrelations of interesting operators [50].

As described in Section 2.7, the overlap Dirac operator involves representing $\epsilon(H_w) = H_w / \sqrt{H_w^2}$. In practice, what is needed is the application of this operator on a vector. One can proceed in several different ways. In four dimensions, it is not practical to store the whole matrix H_w . Therefore standard techniques to deal with the square root of a matrix or exact diagonalization are not considered.

The most efficient method so far is to approximate $\epsilon(H_w)$ as a sum of poles:

$$\epsilon(H_w) \approx g_N(H_w) = H_w \left[c_0 + \sum_{k=1}^N \frac{c_k}{H_w^2 + d_k} \right] \quad (4.2)$$

for some coefficients c_k and d_k . The action of $\epsilon(H_w)$ on a vector then involves a single conjugate gradient with multiple shifts [51]. Since this inversion is needed for every application of the overlap Dirac operator (every application of $\epsilon(H_w)$) it is referred to as the "inner conjugate gradient."

One approximation, called the polar decomposition, has been adapted in this context [52]. In this approximation,

$$\epsilon(z) \approx g_N(z) = \frac{(1+z)^{2N} - (1-z)^{2N}}{(1+z)^{2N} + (1-z)^{2N}} \quad (4.3)$$

and the equation is rewritten as a sum over poles as in Eq. (4.2). Clearly $g_N(z) = g_N(1/z)$ and $g_N(1) = 1$. The error $\epsilon(z) - g_N(z)$ is strictly positive and monotonically decreases from $z = 0$ to $z = 1$. Since $\epsilon(z)$ is scale invariant, the approximation of $g_N(z)$ to $\epsilon(z)$ can be scaled to minimize the error over the region spanned by the eigenvalues of H_w .

Edwards, Heller and Narayanan used another approximation, called the optimal rational approximation [53]: the coefficients are obtained numerically by an optimal fit using the Remez algorithm. The main advantage of the optimal rational approximation over $g_N(z)$ above is the smaller number of poles required for a given accuracy. In practice $N = 14$ was sufficient.

The main limitation of the optimal rational (or any) approximation to $\epsilon(H_w)$ is the range of validity. As discussed in Section 2.6, there is a non-zero density of zero eigenvalues $\rho(0; m)$ of $H_w(m)$ in the super-critical mass region. The small eigenvalues ruin the approximation and increase convergence time in the inner conjugate gradient. To compensate, a small number of the lowest eigenvectors of $H_w(m)$ are calculated and the correct contribution of $\epsilon(H_w)$ is added for the application on a vector. This method allowed computationally tractable calculations of the overlap Dirac operator.

5 Categorical Languages for Parallel Computation

Edwards and Kennedy investigated the use of object-oriented languages for expressing parallel algorithms in an efficient yet portable way. Their goal was to develop within an existing language the framework and data structures which would allow real scientific programs (such as a full dynamical fermion QCD simulation code) to be written such that: (1) the maximum possible efficiency allowed by given hardware should be realizable, (2) the program should be expressed in as modular a way as possible — the higher level code should be written independently of the specification of the underlying data layout and operations — and (3) as much type-checking as possible should be performed to minimize the number of errors in the program. Early attempts in this direction involved the use of a macro preprocessor based upon the UNIX tools *m4* and *ratfor* and is the basis for the current SZIN code used in much of the work done by the SCRI members. This approach was considerably more effective than Fortran, nevertheless, there were many failings. A significant effort was spent in trying to use C++ to express parallel QCD algorithms in a general and portable way. However, the limitations of C++ showed that a language based on category theory such as AXIOM-XL was necessary.

Edwards, Kennedy (now Edinburgh), Watt (West Ontario), and Joo (Edinburgh) have been developing a system for describing parallel computation for QCD and similar problems. This work has been proceeding with support from the Numerical

Analysis Group (NAG) in Oxford. Prototype systems are currently available with more detailed versions under construction.

6 Computer Architecture and Design

Edwards and Kennedy participated in a collaboration with a group of physicists mainly at Columbia university (N. Christ *et al.*) to design teraflop/s-scale computers suitable for computations such as quantum chromodynamics (QCD). The goal of this collaboration was to develop a machine capable of a peak performance of 0.8 Teraflops/s and a true sustained performance of around 35% for QCD [54, 55]. DOE has funded a program to build a machine capable of a peak performance of 0.4 Teraflops and a true sustained performance of around 35% for QCD. The design was directed toward producing a machine which should be as cost-effective as possible.

The 0.4 Teraflops machine at Columbia has in the meantime been built. A 50 Giga flop peak machine was assembled for SCRI and has been in operation since September 1997. Based on this design, the group won the Gordon Bell Prize for Price Performance at SC98 in 1998 [56].

Edwards and Kennedy together with former SCRI postdoc Vranas have written a highly optimized conjugate-gradient inverter that was tested directly on the two-node prototype and obtained 40% of peak. The high level CM-2/workstation code package *SZIN*, developed over the years at SCRI, was ported to the new machine and became the core part of the code that helped the group win the Gordon Bell prize mentioned above.

7 Analytic Calculations

Perturbation theory remains an essential analytic means for controlling the continuum limit in lattice QCD. The ALPHA collaboration has developed a method to compute a running coupling constant non-perturbatively, using the Schrödinger-functional formulation of (lattice) field theory. A lattice perturbation theory computation at two-loop order is required to match this Schrödinger-functional coupling to the coupling defined in the usual $\overline{MS}$ -scheme without significant systematic errors. Bode, together with Weisz (Munich) and Wolff (Berlin), first completed the computation for the pure gauge case [57]. Then they did the calculation for the fermionic part [58]. Besides giving the matching coefficients needed, the calculation also quantifies perturbative discretization errors that arise from working at finite lattice spacing a , which allows to compensate for these errors in numerical Monte Carlo simulations. The calculation of the fermionic contribution was much more challenging than the pure gauge part. It turned out to be more important as well, since the lattice artifacts seem to be much larger in the fermionic sector, making it more important to cancel them.

Kennedy has developed a new method for proving the renormalizability of perturbative field theory (the BPH theorem) [59] and extended this method to proofs of decoupling and over-subtraction (improvement) including the case of lattice theories.

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Supplement to 'Final report to the DOE for the period
8/1/96 to 5/31/00 by the SCRI Theoretical High Energy
Group'

Final Report
June 2002

1 The DØ Experiment

SCRI scientists Linn and Youssef were members of the DØ collaboration since its inception in the early 1980's, and have participated in design, construction, testing, data-taking, and physics analysis. Our early work focused on the design, construction, installation and testing of the liquid-argon calorimeter which achieved superior performance that nearly matched the design parameters. The calorimeter was instrumental in the discovery of the Top quark and in the precision W mass measurement. Later our efforts concentrated on software development and data analysis. During this period we were joined by research associated Xiao, Klatchko, Hirosky, and Chopra. We also co-advised graduate students Madden and Shaffer on Ph.D. dissertations.

1.1 Experimental Support

During the course of data collection all group members contributed to running the experiment by taking shifts. Hirosky served as subconvener for jet analyses within the QCD group, where he coordinated activities concerned with the measurement of jet transverse energies and angular distributions. Linn was subconvener of the QCD photon analysis group. Youssef was the coordinator of event display graphics efforts for Run II. We contributed to the task of Monte Carlo production in DØ, especially within the QCD group. The SCRI AXP cluster was used nearly full time for this purpose, mainly for direct photons, but also for rapidity correlations, and W mass measurements. In addition, the Monte Carlo events were post-processed to include the effect of calorimeter electronic noise, and pileup.

1.2 Software and Computing

As the experiment progressed, we became involved in the software for data analysis and were responsible for design and implementation of the Geant simulation framework. We were responsible for the design and implementation of the analysis techniques used in the Run I photon analysis. Steve Jerger (Michigan State) and Linn developed improved techniques used for the Run I analysis and I undertook a precision calibration of the electromagnetic energy scale of the first calorimeter layer. We improved on the first models of signal and background events which were single photons and neutral mesons by using Pythia events with fragmentation and underlying events. Detector noise and event pileup were included by the addition of real minimum bias events from the data. The energy in the first layer of the calorimeter was used as a discriminant variable and the fraction of photons in the data sample was estimated by fitting admixtures of the signal plus background to the data distributions using a χ^2 minimization procedure.

Youssef developed calorimeter clustering, analysis, event display and electron identification software packages. In particular, event display software has

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been developed for providing detailed 3D event displays of the upgrade systems needed for Run II. He and Klatchko also contributed to the Top analysis.

1.3 Physics Analysis

One primary contribution to the data analysis was in the measurement of direct photons, especially photons at high rapidity which was unique among the Tevatron measurements. The most interesting development in photon physics has been the observation by DØ and CDF of an excess of photons at low E_T . It has been suggested that this is due to additional gluon radiation which is not included in the NLO calculations. This radiation gives rise to a transverse boost of the hard scattering system, which in effect 'smears' the transverse energy resolution of the photon. This smearing will 'soften' the steeply falling photon spectrum, giving rise to an excess of photons at lower E_T when compared to a calculation that does not include this effect. More prosaic explanations such as scale and structure function dependence have also been proposed. It is also of theoretical interest to measure the properties of the photon along with the jets(s) which balance the transverse energy of the event. This analysis was the subject of Madden and Shaffer's dissertations. In the past year the DØ direct photon analysis was completed, subjected to internal review, and published. The analysis combined the integrated luminosity from both parts of Run I, and improved on the Run 1a result by incorporation of a precision calibration of the electromagnetic energy scale. The new analysis also used a more sophisticated model of the background, which was generated using the Pythia event generator. Detector noise and event pileup were included by the addition of real minimum bias events from the data. In the previous analysis, the background was assumed to be isolated pions and eta mesons. The new model suggested the background was more complicated and in general was comprised of higher multiplicity states. Because of uncertainties in the fragmentation model, this technique also yielded a larger systematic error.

Although muon tagging of b-quark jets from top decays is one of the main tools for distinguishing top events from QCD backgrounds, similar electron tagging of b-jets has not been achieved in Q due to difficulties in isolating and track matching low energy electrons and electrons near to a jet axis. Youssef's work has concentrated on achieving similar electron tagging efficiencies and in using this to help extract a top signal from the copious "all-jets" top events from Run I. For central electrons in top events with a CDC track, electron finding efficiencies range from 0.50 for 2-3 GeV electrons up to 0.90 for electrons with energies greater than 15 GeV. This is achieved with a 5% background which is dominated by photon conversions and can mostly be removed by using the central tracking dE/dX measurements and the transition radiation detector. These results are promising for several areas in top analysis and should also be useful as an added signature for mostly muon based B physics cross sections.

Hirosky's interests focused on tests of perturbative quantum chromodynamics (pQCD) in the production of jets of large transverse momenta in $\bar{p}p$ collisions. The good agreement with pQCD over the entire E_T range rules out composite

objects up to mass scales of about 900 GeV. Hirosky was also involved in the study of jet production in diffractive events. Recent theoretical activity has been devoted to exploring the production of jets at large transverse momenta through processes other than the standard parton-parton scattering that is modeled in QCD. The Q measurements will serve as a significant constraint on the parameters in such theoretical models. Hirosky was also involved in the study of hard diffractive processes. There is little understanding of diffractive phenomena, and new experimental results are essential for choosing viable models. Based on his analysis, DØ has presented first evidence for hard single-diffraction in jet production at ~ 1800 GeV. Careful studies of the dynamics of these events can shed light on the nature of the strong color singlet (Pomeron), which is believed to be responsible for the production process. In a related analysis, he searched for evidence of jet production via hard double-Pomeron exchange (HDPE).

1.4 DØ Upgrade

The FSU high energy physics group has taken responsibility for the Silicon Track Trigger (STT) software. The STT combines information from the silicon microstrip detectors (SMD) and the central fiber tracker (CFT). After an event is accepted by the L1 trigger, digitization of SMD elements begins. The first stage of the STT is to convert raw hits into a cluster of hits with a well-defined centroid. The next stage is to associate clusters with tracks found by the CFT. The final step is to fit the track to determine its transverse momentum and vertex displacement. This information is then transmitted to the L2 global processors which combine information from all detectors to make a decision about the event. Horst Wahl is co-project manager while Linn, Chopra, and Repond (FSU postdoc) contribute to the on-line and simulation software. Chopra (now at BNL) has been replaced by W. Lee, who was responsible for on-line monitoring of the system and has also contributed to the simulation. Linn is responsible for time domain simulations of the STT. These queueing simulations follow an event through the different stages of real time processing in the STT. The STT queueing simulation is implemented using the Ptolemy package which is freely distributed by the University of California.