Final Report for “Infrared Fixed Points in Multiflavor Lattice Gauge Theory”
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I. INTRODUCTION

This is the final report for a one year grant that ended on June 30th 2013. The goal of the grant was to apply methods that we have developed with spin and pure gauge models to models with dynamical fermions which are considered as candidates for an alternative to the Higgs mechanism. This project is relevant for the LHC experiment and the Energy Frontier part of the DOE program.

The DOE support has allowed us to provide a 25 percent appointment for a year to Dr. Don Sinclair who has a long-standing expertise in lattice gauge simulations with dynamical fermions. Don Sinclair helped us generating data to study the possible conformal behavior of $SU(3)$ gauge theories with various number of flavors of fundamental quarks using the technique of finite size scaling (Fisher zeros) that we developed for pure gauge theory. The grant also allowed the continuation of Don Sinclair’s work on $SU(3)$ with quark sextets.

Our former graduate student Yuzhi Liu was involved in this project and benefited from the supervision of Don Sinclair. He was supported by several non-DOE sources. He received his Ph. D. in summer 2013 and found a postdoctoral position at University of Colorado Boulder to work on projects related to the research supported by the grant. A new graduate student, Zech Gelzer, now supported as a Teaching Assistant, started to work on related projects and will insure the continuation of the effort at the University of Iowa and the completion of the goals.

The report is organized as follows. Section II provides an overview of the research, its motivations and how it fits in our research program. The work on $SU(3)$ with fundamental quarks is described in section III and the work with sextet quarks in section IV. In Section V, we include a list of publications, talks and graduate students involved.

II. OVERVIEW

The Standard Model is an amazingly good description of the fundamental interactions up to the highest energies probed at collider experiments. The most recent LHC results have provided evidence of a Higgs particle with a mass near 126 GeV, well inside the window $55 \text{ GeV} \leq M_H \leq 135 \text{ GeV}$ predicted from Standard Model radiative corrections and precision physics calculations made years before the LHC results [1]. As there are number of theoretical reasons to doubt of the existence of fundamental scalar particles, a possible alternative to the mass generation by a fundamental scalar particle is to have a composite Higgs made out of fermions interacting strongly via new gauge interactions.

Technicolor theories which are merely scaled-up QCD are not phenomenologically viable. It can be argued that Walking Technicolor theories, where the gauge group and fermion content are such that there is a range of length/mass scales where the running coupling evolves very slowly, might overcome these problems. This typically occurs in situations that can be described as “near conformal”. In this regime, understanding the strong dynamics is

a difficult nonperturbative problem that needs to be properly handled before trying to do realistic model building.

An important aspect of an acceptable theory is that it must describe the light ($m_H \approx \frac{1}{2}v$) Higgs-like particle observed at the LHC. Gauge theories with fermion content such that the theory is asymptotically free, but the 1- and 2-loop contributions to the β -function have opposite signs, are expected to be either conformal or walking.

The location of the conformal windows, the region in parameter space where a nontrivial infra-red fixed point exists, for several families of models have triggered heated discussions. Different numerical and analytical techniques have been applied to QCD-like models with large number of fermion flavors [2–7] or with fermions in higher representations [8–13]. See also [14–16] for recent reviews of results and expectations.

Some examples of near-conformality have been obtained [17] by varying a parameter in such a way that two RG fixed points coalesce and disappear in the complex plane. This motivated us to study extensions of the Renormalization Group (RG) flows in the complex coupling plane [18–20]. In all examples considered, we found that the Fisher’s zeros act as “gates” for the RG flows ending at the strongly coupled fixed point. The Fisher’s zeros are the zeros of the partition function in the complex inverse coupling or inverse temperature plane (later, we use the “ β -plane” terminology). This is a complex extension of the general picture of confinement proposed by Tomboulis [21]. In the case where a phase transition is present, the scaling properties of the zeros [22–27] allow us to distinguish between a first and second order phase transition.

Calculations of RG flows and discrete β functions in lattice gauge theory are notoriously difficult. One of the main questions asked is how many flavors does it take to destroy the confining properties of the theory. For gauge theories, the absence of long-range order (no massless gluons) is associated with confinement. The absence of long-range order also characterizes the 2-dimensional $O(N)$ sigma models with $N \geq 3$.

In [20], we were able to monitor RG fixed points disappearing in the complex inverse temperature (β) plane using the two-lattice matching procedure [28, 29] for Dyson’s hierarchical model [30, 31] with an Ising measure. In this model, the local potential approximation is exact and RG flows can be calculated numerically with good accuracy [32]. The model has a free parameter that plays the role of the dimension and can be tuned continuously. For $D = 3$, the model has a nontrivial Wilson-Fisher fixed point. As we lower D continuously, the fixed point on the real axis moves to the right and eventually disappears at infinity for $D = 2$ in agreement with rigorous results [32].

An important feature that can be observed is that the RG flows approximately follow the Fisher zeros along the separatrix between different basins of attraction. More specifically, in one discrete step, the RG flows approximately go from the zeros at one given number of lattice sites to the zeros for a smaller number of sites as obtained after block spinning. This example shows that the global properties of the RG flows (difficult to calculate) can be inferred from the location of the Fisher’s zeros at successive volumes (easier to calculate). Similar observations were made for the $2D$ $O(N)$ non-linear sigma models in the large- N limit [19].

We have used the density of states $n(S)$, the exponential of the entropy which describes the relative number of configurations with a given action S , to analyze the Fisher’s zeros of lattice gauge models. The pure-gauge partition function can be written as the Laplace transform of the density of states. which allows us to calculate Z for complex values of

β . In the case of $D = 4$ pure gauge $SU(2)$, numerical results were checked with existing expansions [33], and it was found that the zeros stay away from the real axis as the 4-volume increases [18]. In the case of $D = 4$ pure gauge $U(1)$ theory [34], we used the multi-canonical algorithm developed by Berg and Bazavov [35] to construct the density of states. For small volumes, we were able to locate the lowest zeros with a precision of order 10^{-5} . The imaginary part of the zeros scales like $L^{-3.07}$, or $\nu = 0.326$ in the apparently consistent second-order phase transition hypothesis. However the zeros from higher volumes show that the scaling is “rolling” and ν is decreasing with volumes. With this work we developed the technical tools to deal with the more complicated case of gauge theories with fermions that is the main focus of the grant for which this report is written.

III. FISHER ZEROS IN QCD WITH 4 TO 12 FUNDAMENTAL QUARKS

D. Sinclair has developed a code to simulate $SU(3)$ with 2 and 3 fermion flavors in order to study finite temperature QCD. The lattice action is based on the unimproved staggered action and the gauge field action is the standard Wilson action. The effects of improvement are under study (see below). In order to simulate N_f fermion flavors, the following fermion action is used:

$$S_f = \sum_{sites} \chi^\dagger \{[\not{D} + m][-\not{D} + m]\}^{N_f/8} \chi. \quad (1)$$

In the Rational Hybrid Monte Carlo (RHMC) algorithm used in Ref. [36], the fractional power of the matrix has been replaced by rational approximations. We have used M. Clark’s public code based on the Remez algorithm to get the optimal rational approximation in a specified range and we have calculated the approximants for N_f up to 16. We were able to tune the molecular dynamics time in order to reach the optimum acceptance rate for N_f up to 12. One particularly challenging task was to modify the existing code by including multiple fermion forces terms to ensure that the code works efficiently in the strong coupling region for large number of fermion flavors. We also made numerical experiments for non-integer N_f and found that computationally, there seems to be no issues and that standard average quantities seem to vary smoothly when N_f is changed continuously. This has been done with our graduate student Yuzhi Liu who did excellent work and graduated in summer 2013.

We have conducted extensive runs for $N_f = 4$ and $N_f = 12$ at NERSC Hopper and Carver supercomputers. The core time needed to generate 5000 trajectories for a 4^4 volume is around 3.5 hours and the corresponding time for 4×8^3 and 4×16^3 volume is about 48 hours and 360 hours. Even at small volume, one can see that the crossover behavior that seems clear for 4 flavors sharpens significantly as the number of flavors increases from 4 to 12 as shown in Fig. 1. Calculations at non integer values of N_f are possible as we are using the rational approximation and seem to interpolate smoothly between the integer values. For $N_f = 12$, there is a discontinuity in the average plaquette and $\langle \bar{\Psi}\Psi \rangle$ at approximately the same, volume dependent, values of β . What could be interpreted as a finite temperature transition for small value of the length of the temporal size in lattice units N_t , seems to turn into a first order bulk transition at a finite value of β . This situation is illustrated in Figs. 2 and 3. We were able to confirm the nature of the transition (first order) by using the scaling of the the lowest zeros at different L : they pinch the real axis at a L^{-4} rate as

FIG. 1. Average plaquette for integer and non-integer N_f ; $V = 4^4$; $m = 0.02$.

FIG. 2. Plaquette $\langle \bar{\psi}\psi \rangle$ discontinuities for various lattices. 8 4 means a $8^3 \times 4$ lattice.

FIG. 3. Polyakov's loop (time-periodic Wilson's line) for various lattices. 8 4 means $8^3 \times 4$ lattice.

FIG. 4. Fisher's zeros for $N_f = 4$ and $N_f = 12$ for some L^4 lattices (left). For $N_f=12$, the lowest zeros pinch the real axis like L^{-D} (right).

FIG. 5. Schematic representation of the RG flows. The bare parameters are in the purple plane where the “other” parameters induced by renormalization are zero.

illustrated in Fig. 4.

More generally the Fisher zeros can be used to reconstruct the Renormalization Group (RG) flows. We expect these flows to have a global behavior in a generic coupling, mass and “others” (induced by renormalization) space schematically displayed in Fig. 5. The L^{-4} behavior discussed above is related to a small part of these flows namely at the boundary between the chirally broken and chirally symmetric region at small mass. Increasing the mass should at some point make this separation disappear. Graduate student Zech Gelzer has been searching for the end point as shown in Fig. 6. Larger masses seem required to reach this endpoint. There remain important questions that we are presently working on. Will the Fisher's zero pinch the real axis like L^{-2} ($\nu=1/2$, mean field for a free scalar) instead

of L^{-4} near the end point (for $m = m_c$)? Is it possible to find a hint of the IR fixed point from the behavior of the zeros over a broader β interval as a function of m ? As the approach of the possible infrared fixed point in the massless limit proceeds along irrelevant directions, the process may be very slow and require very large volumes to be observed.

Another important question is the effect of improvement on the flows and the zeros. Zech Gelzer is now running a code where the effect of the improvement can be changed adiabatically and plan to study the phases changes and the effect on the zeros. This is a hybrid Monte Carlo code for improved staggered fermions with nHYP smearing. The code is based on the widely used MIMD Lattice Computation (MILC) Collaboration software. The code uses Omelyan integrator with multiple time scales and mass preconditioning to optimize the performance. It can simulate systems with 4, 8, 12 and 16 fundamental fermions at non-zero and zero quark masses. The smearing parameters and steps can be adjusted at will, which means one could change the fermion action adiabatically from smeared one to the naive non-smeared one used before. It also has the option to add an adjoint plaquette term to the gauge action with either positive or negative coefficient. This work is being done with the UC Boulder group.

In general for $SU(3)$ with 8 to 12 fundamental quarks or 2 to 3 sextets, the approach of an hypothetical conformal fixed point in the massless limit requires large sizes in space and time and patience for the researcher. This motivated us to develop non Monte Carlo methods where exponentially large volumes can be reached. These methods are based on the tensor RG method and apply to most models [37, 38] studied by lattice gauge theorists. Recent numerical applications for spin models have been very successful.

FIG. 6. Average plaquette and $\langle \bar{\psi}\psi \rangle$ for $N_f = 12$, $V = 4^4$ and various masses.

IV. QCD WITH COLOUR-SEXTET STAGGERED QUARKS

A candidate theory for a composite Higgs is (techni-)QCD with 2 massless (techni-)color-sextet (techni-)quarks, which could be either walking or conformal. We contrast this theory with the 3-(techni-)flavor version, which is expected to be conformal. QCD with 2 color-sextet quarks has 3 Goldstone bosons – the correct number to give mass to the W s and Z with none left over. Because chiral symmetry breaking and confinement occur at very different scales, one expects (techni-)hadrons associated with both scales.

Don Sinclair has studied extensively QCD with 2 color-sextet quarks as a model for walking Technicolor. He used lattice gauge theory simulations (RHMC) at finite temperature. The goal is to determine if the massless theory is QCD-like (confining, with spontaneously-broken chiral symmetry) with a slowly varying coupling (walks) or if it is a conformal field theory. This can be done by simulating the theory at finite temperature and observing how the coupling at the chiral-symmetry restoration temperature depends on the temporal extent N_t of the lattice (in lattice units). If the theory is QCD-like, this coupling should approach zero in the large N_t limit in the manner predicted by asymptotic freedom. If it is conformal, this coupling should approach a finite value in this limit, i.e. the transition would be a bulk transition.

Since it is difficult if not impossible (see Fig. 7) to extrapolate either the unsubtracted or subtracted chiral condensates to zero quark mass with sufficient reliability to determine the position of the chiral-symmetry-restoration phase transition accurately, the value of β_χ will be estimated from the peaks in the chiral susceptibility:

$$\chi_{\bar{\psi}\psi} = \frac{V}{T} [\langle (\bar{\psi}\psi)^2 \rangle - \langle \bar{\psi}\psi \rangle^2]$$

extrapolated to $m = 0$.

FIG. 7. Chiral condensates and Polyakov Loops on a $24^3 \times 12$ lattice.

FIG. 8. Chiral susceptibilities on a $16^3 \times 8$ and a $24^3 \times 12$ lattice.

For $N_f = 2$ and $N_t = 8$, the work was done mainly on a $16^3 \times 8$ lattice and also on a $24^3 \times 8$ lattice at $\beta = 6.7$ and $\beta = 6.9$, both with $m = 0.0025$. Other simulations were performed at $m = 0.02$, $m = 0.01$, $m = 0.005$, and $m = 0.0025$. In the neighbourhood of the chiral transition, $6.6 \leq \beta \leq 6.8$, runs of 50,000 length-1 trajectories were done at $m = 0.02$, $m = 0.01$, and $m = 0.005$ for each β and m . At $m = 0.0025$ 100,000 trajectories for each β in this range were used. The position of the peak for $m = 0.0025$ is taken as the estimate of β_χ . This gives $\beta_\chi = 6.69(1)$. These susceptibilities are shown in Fig. 8.

For $N_t = 12$, simulations were done with $N_t = 12$ on $24^3 \times 12$ lattices, at quark masses $m = 0.01$, $m = 0.005$, and $m = 0.0025$. In the neighbourhood of the chiral transition $6.6 \leq \beta \leq 6.9$ simulations were performed at β s spaced by $\delta\beta = 0.02$. So far we have simulated 25,000 – 50,000 length-1 trajectories at each (β, m) in this range (with 2 exceptions). Fig. 7 shows the unsubtracted chiral condensates $\langle\bar{\psi}\psi\rangle$ measured in these simulations. Note that, although these suggest that the condensate will vanish in the chiral limit for β sufficiently large, any attempt to extrapolate to $m = 0$ to estimate β_χ would be plagued with systematic uncertainties. Using subtracted condensates improves the situation, but not sufficiently to extract β_χ accurately. These susceptibilities are shown in Fig. 8. Both the $m = 0.005$ and $m = 0.0025$ susceptibilities show peaks. While the data is consistent with there being little mass dependence of the position of the peaks, it is not yet compelling. More statistics is needed. The best estimate of β_χ from the current data is $\beta_\chi = 6.78(2)$.

This implies that:

$$\beta_\chi(N_t = 12) - \beta_\chi(N_t = 8) = 0.09(2)$$

compared with the 2-loop perturbative prediction

$$\beta_\chi(N_t = 12) - \beta_\chi(N_t = 8) \approx 0.12$$

The critical values are summarized in the Table I.

N_t	β_d	β_χ
4	5.40(1)	6.3(1)
6	5.54(1)	6.6(1)
8	5.65(1)	6.69(1)
12	5.75(5)	6.78(2)

TABLE I. $N_f = 2$ deconfinement and chiral transitions for $N_t = 4, 6, 8, 12$.

FIG. 9. Chiral condensates and chiral susceptibilities on $24^3 \times N_t$ lattices at $\beta = 6.9$.

Simulations at fixed beta and $24^3 \times N_t$ were also performed for various N_t , with $N_t \leq 24$ at fixed β , to search for evidence of a transition back to the chirally broken phase as N_t is increased. $\beta = 6.9$ was chosen. If the evolution of β_χ is governed by the 2-loop β -function, $\beta_\chi \approx 6.9$ for $N_t = 18$. Hence we should see evidence for the chiral transition as N_t is increased. Fig. 9 shows the unsubtracted and subtracted chiral condensates as functions of N_t for these runs. Following Fodor *et al.*, one can define a subtracted chiral condensate by:

$$\langle \bar{\psi}\psi \rangle_{sub} = \langle \bar{\psi}\psi \rangle - \left(m_V \frac{\partial}{\partial m_V} \langle \bar{\psi}\psi \rangle \right)_{m_V=m}$$

where m_V is the valence quark mass. We should try other schemes. Fig. 9 shows the chiral susceptibilities for these runs.

We searched for Fisher zeros using various plaquette distributions for $N_f=2$ and found that the zeros appeared at the limit of the radius of confidence of the procedure indicating a QCD like behavior. This is illustrated in Fig. 10.

Simulations with $N_f = 3$ and $N_t = 8$ were performed on $16^3 \times 8$ lattices at $m = 0.01$ and $m = 0.005$. Fig. 11 shows the chiral susceptibilities for these runs. From this the best estimate is $\beta_\chi = 6.38(2)$, somewhat larger than that for $N_t = 6$. The increase in β , $\beta_\chi(N_t = 8) - \beta_\chi(N_t = 6)$ is appreciably larger than the ≈ 0.0025 predicted by 2-loop pertur-

FIG. 10. Search for zeros for two sextet. The circle is the boundary of the region of confidence of the calculation.

FIG. 11. Chiral susceptibilities for $N_f = 3$ on a $16^3 \times 8$ lattice.

bation theory. Nor can we see any evidence that $\beta_\chi(N_t)$ is approaching a non-zero constant as $N_t \rightarrow \infty$ as expected, since this theory is expected to be conformal. We will therefore need to perform simulations at $N_t = 12$.

V. PUBLICATIONS, PRESENTATIONS AND GRADUATE STUDENTS INVOLVED

Publications

- Fisher zeros and conformality in lattice models Yannick Meurice, Alexei Bazavov, Bernd A. Berg, Daping Du, Alan Denbleyker, Yuzhi Liu , Donald K. Sinclair , Judah Unmuth-Yockey, and Haiyuan Zou, Fisher zeros and conformality in lattice models, arXiv:1210.6969, Oct 2012. 7 pp. , Published in PoS LATTICE2012 (2012) 229
- D. K. Sinclair, J. B. Kogut, QCD with colour-sextet quarks, arXiv:1211.0712, Published in PoS(Lattice 2012)026 (2012)

Talks related to the project

- D. Sinclair, QCD with colour-sextet quarks, Lattice 2012, Cairns, Australia, June 2012
- D. Sinclair, Further studies of QCD with sextet quarks, Lattice 2013, Mainz, Germany, July 2013 <http://www.lattice2013.uni-mainz.de/presentations/4F/Sinclair.pdf>
- D. Sinclair, Further studies of QCD with sextet quarks, CP3, Odense, Denmark, August 2013. <http://cp3-origins.dk/video/107670010>
- Y. Meurice, Fisher zeros and conformality in lattice models, Lattice 2012, Cairns, Australia, June 2012
- Y. Meurice, KITPC Program “Critical Behavior of Lattice Models,” July-August 2012
- Y. Meurice, Continuum limits of 12 flavor QCD, APS March meeting 2013,
- Y. Meurice, BNL, Fisher’s zeros in spin/gauge models and beyond the standard model, April 2013
- Y. Meurice, Stony Brook, Dyson instability beyond the standard model, April 2013
- Y. Meurice, Baruch College, Alternatives to Monte Carlo, April 2013
- Y. Meurice, Syracuse, Lattice models near conformality, April 2013
- Yuzhi Liu, Fisher’s zeros for $SU(3)$ with N_f flavors and RG flows, Lattice 2013, Mainz, Germany, July 2013 <http://www.lattice2013.uni-mainz.de/presentations/3F/Liu.pdf>

Graduate students involved

- Yuzhi Liu, PhD, July 2013, “Renormalization Group and Phase Transitions in Spin, Gauge and QCD-like Theories,” position in September 2013 as a postdoc at the University of Colorado, Boulder. He was supported by Vice-President of Research internal grant in 2011-2012 and by a URA fellowship from August 2012 to August 2013.
- Zech Gelzer, Teaching Assistant, PhD expected in 2017.

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