Towards the Continuum Limit of Lattice Gauge Theory with Dynamical Fermions

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Simulations of Su(3) lattice gauge theory with four species of light quarks show a large peak in the bulk specific heat near $\beta = 6/g^2 \approx 5.10$ separating strong and weak coupling. $\langle\bar{\psi}\psi\rangle$ satisfies asymptotic-freedom scaling for $\beta = 6/g^2 \gtrsim 5.10$ and $\langle\bar{\psi}\psi\rangle^{1/3}/\Lambda_{\overline{\rm MS}} = (2.6 \pm 0.1)(4\pi^2\beta/25)^{4/25}$ ($\overline{\rm MS}$ denotes the modified minimal-subtraction scheme). Finite-temperature simulations on a 6×10^3 tice show a smooth but rapid crossover at $T/\Lambda_{\overline{\rm MS}} = 2.14 \pm 0.10$. We find no evidence for metastable states.

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The first step toward solving quantum chromodynamics numerically by lattice methods consists in understanding its scaling laws and phase diagrams for zero and nonzero physical temperatures. The approach to the continuum limit is controlled by asymptotic freedom which states that physical mass scales as the lattice Λ parameter should depend on the lattice coupling $\beta = 6/g^2$ as

$$a\Lambda_L = (8\pi^2\beta/25)^{231/625}\exp(-4\pi^2\beta/25) \qquad (1)$$

when g^2 approaches zero. Equation (1) applies to the SU(3) gauge group coupled to four species of massless quarks. In a simulation of lattice gauge theory Eq. (1) can be verified most easily by the study of local quantities such as the chiral order parameter $\langle\bar{\psi}\psi\rangle$ or the temperature at which chiral symmetry is restored when quantum chromodynamics is heated. Equation (1) also applies to the masses of hadronic states, but precise measurements of composite propagators on the lattice are particularly difficult. One needs improved algorithms which can relax the long-wavelength modes of the lattice theory efficiently so that statistical errors do not overwhelm the determination of the long-distance tails of the propagators. There are proposals to that,[1] but in this Letter I report relatively accurate measurements of local observables only. I will use the tuned-hybrid-stochastic-differential-equation approach in this study.[2] This algorithm is much more efficient than the naive Langevin equation.[3] It is also subject to straightforward error analysis which eludes the naive pseudofermion Monte Carlo method.[4] The hybrid algorithm has been described elsewhere,[2] and so this Letter will concentrate on results of physical interest.

I first simulated the lattice theory on a symmetric 8^4 lattice to understand its crossover from strong to weak coupling. The average of the plaquette variable S_0, tr$UUUU$ (the Wilson action), was measured for $\beta = 5.00$, 5.05, 5.075, 5.10, 5.15, 5.20, 5.25, and 5.30 to an accuracy of one part in 500 at each point. Bare-fermions masses of $m = 0.10$, 0.07, and 0.05 (in lattice units) were used at each β value. The bulk specific heat, $C = -dS_0/d\beta$, was computed by finite differencing, $-\Delta S_0/\Delta\beta$, and the results are shown in Fig. 1. We observe a sharp peak at $\beta \approx 5.10$ separating strong- and weak-coupling behaviors. This phenomenon reminds us of the crossover in the pure gluon theory.[5] The vacuum polarization provided by the fermions has in large measure simply shifted the specific-heat peak of the pure gluon theory to stronger coupling. This is a nonperturbative, nonuniversal lattice effect which bodes evil for Eq. (1)—large values of β (certainly larger than 5.10) are necessary for this perturbative renormalization group result to apply. To investigate this, $\langle\bar{\psi}\psi\rangle$ was measured in the same simulation, its values were extrapolated to $m = 0$ for each β value, and the result was plotted versus β as shown in Fig. 2.

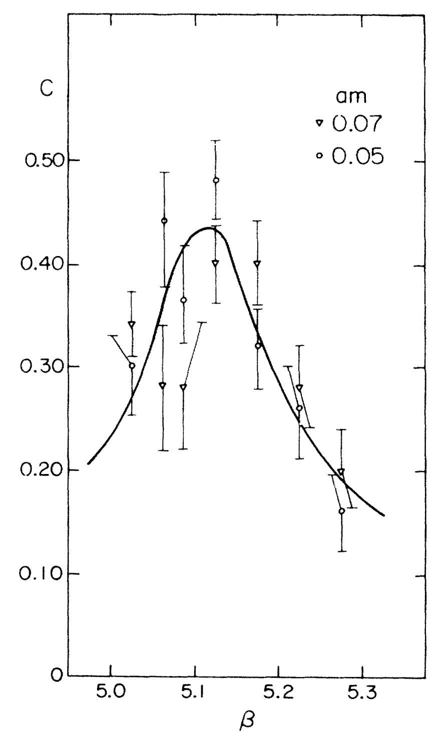

FIG. 1. The bulk specific heat, $C = -dS_0/d\beta$. Typical error bars are shown.

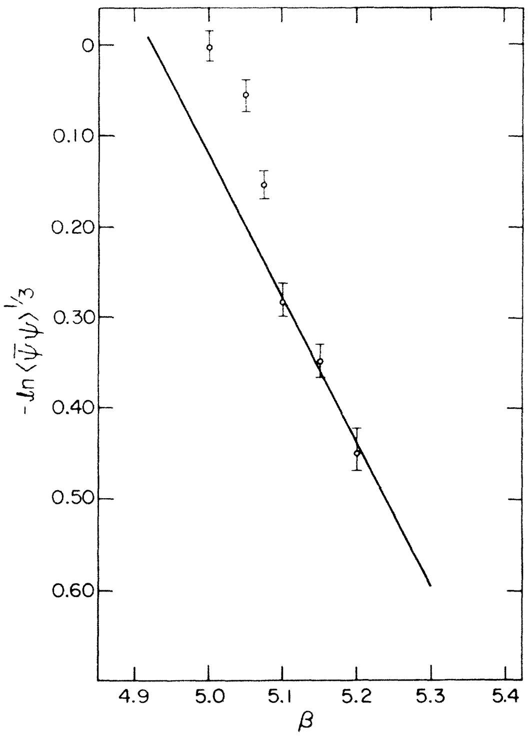

FIG. 2. $\langle\bar{\psi}\psi\rangle$ scaling curve after the linear $m\to 0.00$ extrapolation.

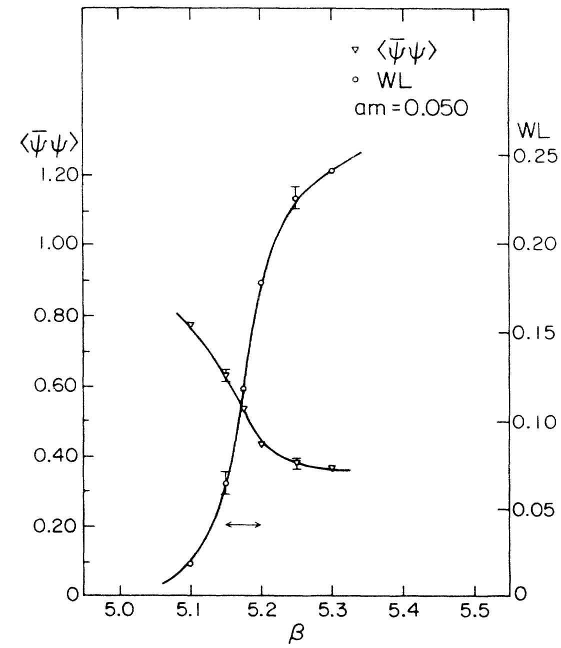

FIG. 3. $\langle\bar{\psi}\psi\rangle$ and Wilson-Polyakov line expectation values on a 6×10^3 lattice for $m=0.05$. Typical error bars are shown.

In particular, the small-g^2 scaling law for $\langle\bar{\psi}\psi\rangle$ reads, when we account for its anomalous dimension,

$$\langle\psi\psi\rangle^{1/3}=R(4\pi^2\beta/25)^{4/15}\Lambda_L, \quad (2)$$

where R is a dimensionless constant determined by the simulation. The figure shows that the scaling law Eq. (2) applies quite well for $\beta\gtrsim 5.10$ although the error bars on $\langle\bar{\psi}\psi\rangle$ are considerable. If we write Eq. (2) in terms of $\Lambda_{\overline{\rm MS}}$ ($\overline{\rm MS}$ denotes the modified minimal-subtraction scheme), we find ($\Lambda_{\overline{\rm MS}}/\Lambda_L\approx 76.44$)

$$\langle\bar{\psi}\psi\rangle^{1/3}=(2.6\pm 0.1)(4\pi^2\beta/25)^{4/25}\Lambda_{\overline{\rm MS}}. \quad (3)$$

Simulations of the pure gluon theory on 8^4-point lattices predict[6]

$$\langle\bar{\psi}\psi\rangle^{1/3}=(3.8\pm 0.5)(4\pi^2\beta/33)^{4/33}\Lambda_{\overline{\rm MS}} \quad \text{(pure gluon theory)}. \quad (4)$$

Equations (3) and (4) will be discussed further below.

Figures 1 and 2 indicate that continuum physics can be read off lattice simulations of this theory only if β is chosen larger than 5.10. Presumably a more accurate determination of $\langle\bar{\psi}\psi\rangle$ would show a gradual approach to scaling behavior as $\beta\to\infty$ with computable corrections to scaling coming from the leading nonrenormalizable operators in the operator-product expansion of the lattice action. Nonetheless, Fig. 2 is a nontrivial test of the hybrid algorithm and it indicates that some physical scales of hadronic physics are accessible to present-day simulations.

However, the large scaling violations shown in Figs. 1 and 2 for $\beta\approx 5.10$ indicate that all past studies of the thermodynamics of the theory have not been in the scaling region. Recall that the theory has been simulated on a 4×8^3 lattice and a rapid crossover from hadronic to quark-gluon–plasma behavior was found at $\beta=5.025\pm 0.025$.[7] These "finite temperature" results were certainly influenced by the bulk crossover phenomenon seen in Fig. 1. The sharp peak in the bulk specific heat may, in fact, be the cause of some groups' contention that a hard first-order finite-temperature transition exists even when fermion vacuum polarization is included in the dynamics.[8] To clarify this issue I simulated the theory at finite temperature on a larger lattice, 6×10^3, at relatively small bare-quark masses, $m=0.10$, 0.065, and 0.050. Typically 1.5×10^4 iterations of the hybrid stochastic differential equations were executed with a discrete time step of $dt=0.02$ at each β and m. At $m=0.050$ data were taken at $\beta=5.30$, 5.25, 5.20, 5.175, 5.15, and 5.10. The observables included $\langle\bar{\psi}\psi\rangle$, the Wilson-Polyakov line WL, the quark and gluon energy densities, and the Wilson-Polyakov line correlation functions. The data at $m=0.050$ for $\langle\bar{\psi}\psi\rangle$ and the WL are shown in Fig. 3. We note a rapid but smooth crossover as β varies from 5.15 to 5.20. The $\langle\bar{\psi}\psi\rangle$ and WL curves are, in fact, considerably smoother than those measured on a 4×8^3 lattice. In Fig. 4 I show the result of two long runs of the algorithm at $\beta=5.175$, one be-

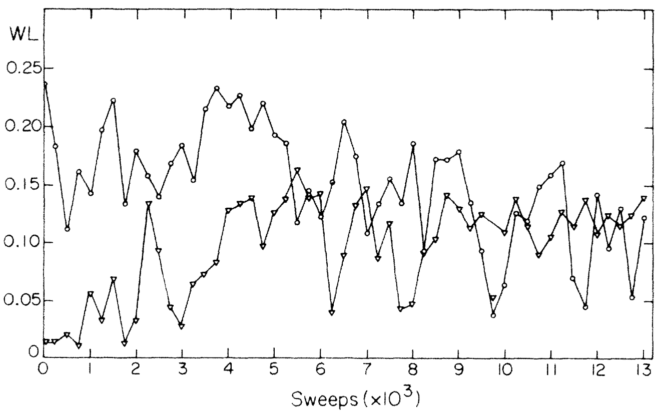

FIG. 4. Wilson-Polyakov line measurements at $\beta = 5.175$ beginning with a cold and a hot start.

ginning with a equilibrium state prepared at $\beta = 5.25$ (hot) and the other at $\beta = 5.10$ (cold). The WL's of both the hot and cold starts evolve smoothly to the equilibrium value characteristic of $\beta = 5.175$. No evidence for metastability is found. Similar studies of $\langle\bar{\psi}\psi\rangle$ and S_0 confirm this result.

Finally we can estimate the physical temperature of this narrow crossover region. At $m = 0.050$ the crossover occurs at $\beta = 5.175$ which is in the scaling region of Fig. 2. Since $N_t = 6$, the physical temperature of the lattice is $aT = \frac{1}{6}$, where a is the lattice spacing. In terms of Λ_L, $\beta = 5.175 \pm 0.025$ corresponds to $T/\Lambda_L = 210 \pm 8$ which can be expressed in terms of $\Lambda_{\overline{\text{MS}}}$,

$$T/\Lambda_{\overline{\text{MS}}} = 2.75 \pm 0.10 \quad (m = 0.050). \tag{5a}$$

It is also interesting to take the $m = 0.10$, 0.65, and 0.050 data and extrapolate them to massless quarks. The crossover at $m = 0.10$ occurs at $\beta = 5.325 \pm 0.025$, for $m = 0.065$ at $\beta = 5.225 \pm 0.025$ and for $m = 0.050$ at $\beta = 5.175 \pm 0.025$. These three points extrapolate linearly to $m = 0.00$ where $\beta = 5.010 \pm 0.025$. Using Eq. (1) we then have

$$T/\Lambda_{\overline{\text{MS}}} = 2.14 \pm 0.10 \quad (m = 0.00 \text{ limit}), \tag{5b}$$

where the uncertainty reflects the widths of the crossover regions in the data, and does not account for the systematic uncertainty in the extrapolation procedure. Since the extrapolation takes us from $\beta = 5.175$ to $\beta = 5.01$ which does not lie in the scaling region, the theoretical uncertainty in Eq. (5b) is considerable. Presumably, the true $N_t = 6$ estimate of $T/\Lambda_{\overline{\text{MS}}}$ for light quarks lies between Eqs. (5a) and (5b).

It is interesting to compare Eq. (5b) to estimates of the hard deconfining transition in the pure gluon theory at $N_t = 6$,[9]

$$T/\Lambda_{\overline{\text{MS}}} = 2.12 \quad (\text{pure gluon theory}). \tag{6}$$

Remarkably, the effect of fermion vacuum polarization cancels out of the ratio $T/\Lambda_{\overline{\text{MS}}}$. This is also roughly true for other physical quantities such as $T/\langle\bar{\psi}\psi\rangle^{1/3}$,

$$\begin{aligned} T/\langle\bar{\psi}\psi\rangle^{1/3} &= (0.56 \pm 0.10)(4\pi^2\beta/33)^{-4/33} \quad (\text{pure gluon theory}), \\ T/\langle\bar{\psi}\psi\rangle^{1/3} &= (0.85 \pm 0.05)(4\pi^2\beta/25)^{-4/25} \quad (\text{four quark species}). \end{aligned} \tag{7}$$

The anomalous factors in Eq. (7) are close to unity for the couplings accessible to lattice simulations and are included here only for completeness.

Equations (3), (5), and (7) are encouraging results. The temperature of the crossover region and the magnitude of $\langle\bar{\psi}\psi\rangle$ in the theory with light dynamical quarks look very reasonable physically. However, in light of Ref. 9, which shows that there are nonnegligible scaling violations at $N_t = 6$ in the pure gluon theory, we must expect systematic small changes in Eq. (5b) as larger lattices are studied. Much more accurate measurements and renormalization-group and/or finite-size-scaling studies will be required to refine the results presented here. In addition, general symmetry arguments suggest that the chiral-symmetry–restoring transition at finite temperature should be a fluctuation-induced first-order one.[10] Perhaps when larger lattices, which better approximate the space-time continuum, are studied this effect will be seen.

A lengthier account of this research, complete with tables of simulation data, will be presented elsewhere.

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