PHYSICAL REVIEW D VOLUME 41, NUMBER 2 15 JANUARY 1990

QCD thermodynamics with eight time slices

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(Received 31 August 1989)

Preliminary simulations of lattice QCD with two flavors of Kogut-Susskind quarks with masses of $0.025a^{-1}$ and $0.0125a^{-1}$ locate the expected crossover from the low-temperature regime of ordinary hadronic matter to the high-temperature chiral-symmetric regime. These calculations are insufficient to distinguish between a rapid crossover and a true phase transition.

I. INTRODUCTION

Numerical simulations of lattice QCD have provided some of our clearest insights into the behavior of the theory at high temperature. Extensive simulations have been carried out with four Euclidean time slices ($a=1/4T_c$), using two and four flavors of staggered quarks, to investigate the phase structure of QCD as a function of quark mass and temperature.[1] The picture that emerges is that for low- or zero-mass quarks there is a phase transition between the low-temperature state of ordinary hadronic matter and the high-temperature state in which chiral symmetry is realized explicitly. As the quark mass increases this transition disappears, leaving a rapid crossover as a function of temperature. For still larger masses a transition reappears and at infinite quark mass this transition becomes the much better studied "deconfinement" phase transition of pure-glue QCD. Physical observables which probe the nature of the high-temperature phase have also been studied with four time slices[2] and low-temperature simulations at similar bare parameters have been used to estimate the physical lattice spacing and hence the transition temperature.[3] However, if we are to obtain reliable quantitative results it is necessary to work at much smaller lattice spacings or, equivalently, many more time slices than have been studied to date. Because the phase-transition temperature (in units of the ρ or nucleon mass) is lower for full QCD than for the pure-glue theory, we will require more time slices to study the transition for full QCD than were required to study the pure-glue QCD transition at the same lattice spacing. (We estimate that in full QCD around 14 time slices will be required to see "asymptotic scaling," the agreement of the dependence of the lattice spacing on g with the two-loop perturbative β function.)

As a step in the direction of smaller lattice spacing we have carried out simulations of QCD with two flavors of Kogut-Susskind quarks on a $12^3\times 8$ lattice. As usual, we have used quark masses larger than the real-world u and d masses. Even so, these simulations are extremely time consuming and the runs are much shorter than we would like. Therefore, the amount of analysis which is justified is limited, and we will simply present the time histories and two plots showing the averages of the Polyakov loop and $\bar{\psi}\psi$ as a function of $6/g^2$.

II. RESULTS

We have used the hybrid, or refreshed-molecular-dynamics, algorithm[4] as described in Ref. 5. In this algorithm the system evolves in "simulation time" in such a way that once it has come to equilibrium the probability distribution of configurations is the desired $\det M(U)\exp(-S_g)$. The normalization of the simulation time is defined by the equations

$$\begin{aligned}&\dot{U}=iHU,\quad H=\sum_a \lambda_a h_a,\\&\mathrm{Tr}\lambda_a\lambda_b=2\delta_{ab}\ ,\\&\langle h_a h_b\rangle=\tfrac{1}{2}\delta_{ab}\ .\end{aligned}\tag{1}$$

U is a link matrix, and the λ_a are the standard generators of SU(3). This normalization varies throughout the literature. With a quark mass, m_q of $0.025a^{-1}$ we used a time step of 0.02, and at $m_q=0.0125a^{-1}$ a time step of 0.01. The "momenta" H were refreshed every 0.5 units of simulation time.

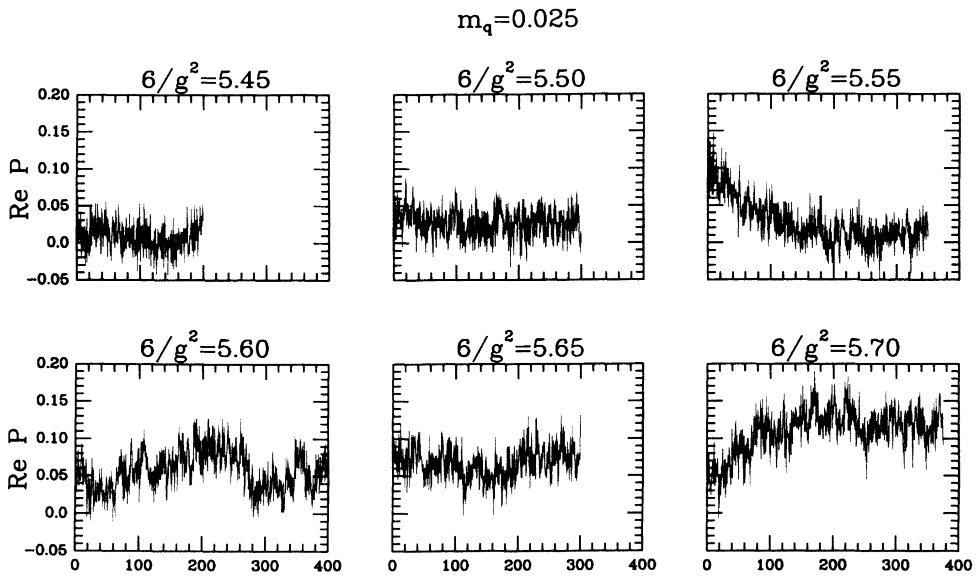

FIG. 1. Time histories of the real part of the Polyakov loop for $m_q = 0.025$.

The effects of the quarks on the motion of the link matrices requires repeated computation of $M^{-1}u$, where M is the fermion hopping matrix and u is a random vector. This is done by using the conjugate-gradient method to compute $(M^{\dagger}M)^{-1}M^{\dagger}u$. The conjugate gradient was stopped when the normalized residual $\sqrt{R^2/V}$, where V is the four-dimensional volume of the system, reached a predetermined value. In our normalization the mean-squared magnitude of u is $\frac{3}{2}V$. At quark mass of $0.025a^{-1}$ we used a stopping criterion of $\sqrt{R^2/V} < 0.0025$, and for $m_q = 0.0125a^{-1}$ we required $\sqrt{R^2/V} < 0.00125$. The number of conjugate-gradient iterations required to reach this residual depends strongly on whether the system is in the hot or cold phase. For example, at $m_q = 0.025a^{-1}$ about 158 iterations were required at $6/g^2 = 5.45$ and 91 iterations at $6/g^2 = 5.65$. For $m_q = 0.0125a^{-1}$ these numbers were 334 and 116, respectively.

Our investigations on small lattices[6] together with our ideas on how these parameters should scale lead us to believe that this step size and conjugate-gradient residual are reasonable. In addition, we have performed tests on a 12^4 lattice at similar parameters suggesting that the effects of this step size and stopping criterion on the plaquette and $\bar{\psi}\psi$ are small, though measurable.

In Fig. 1 we show the simulation time histories of the

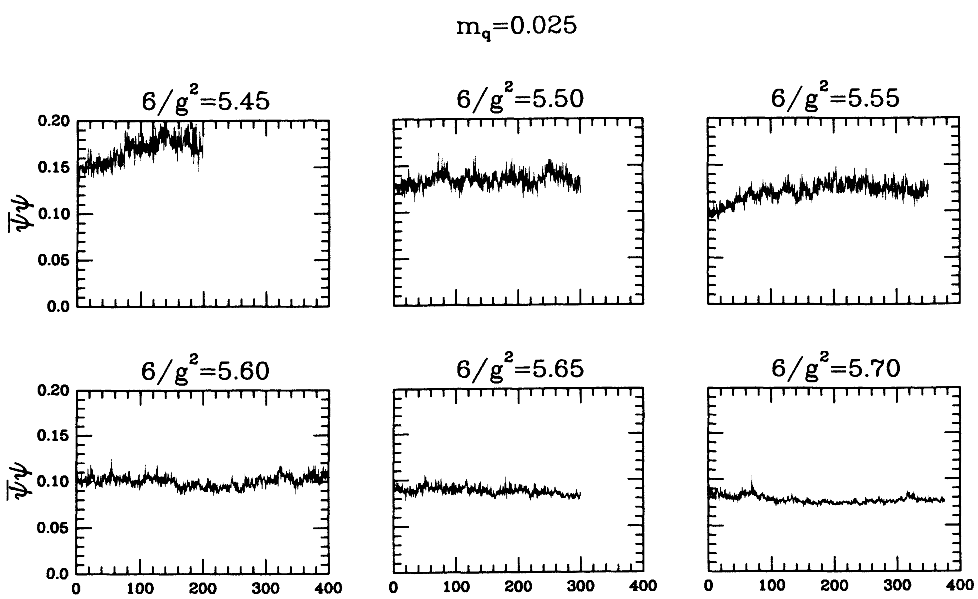

FIG. 2. Time histories of $\bar{\psi}\psi$ for $m_q = 0.025$.

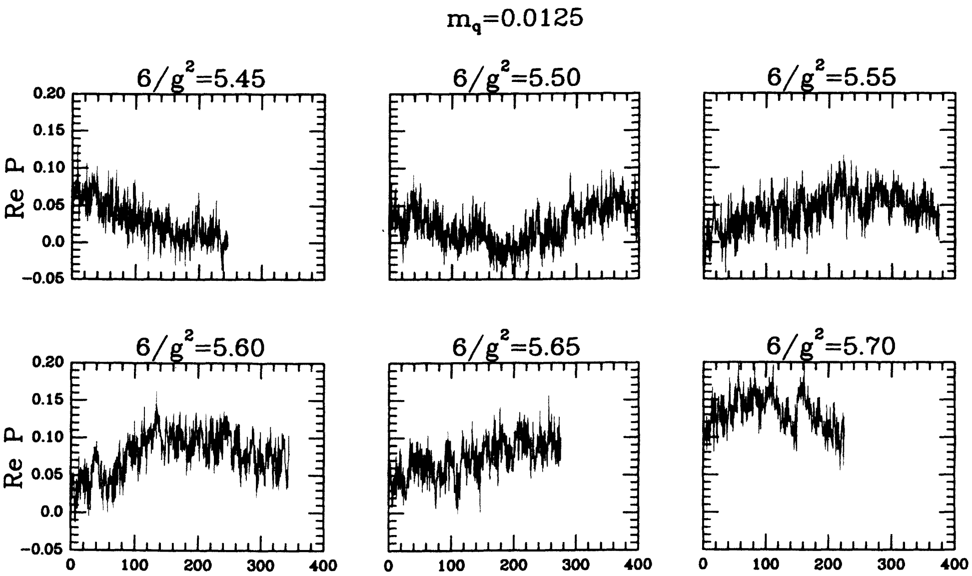

FIG. 3. Time histories of the real part of the Polyakov loop for $m_q = 0.0125$.

real part of the Polyakov loop in our runs at $m_q = 0.025a^{-1}$. Here we normalize to three on a completely ordered lattice. Figure 2 shows $\bar{\psi}\psi$ for these same results. In normalizing $\bar{\psi}\psi$ we give the sum over the three colors and two flavors, and choose the normalization of the fermion hopping matrix M so that its diagonal elements are $2m_q$. Figures 3 and 4 show time histories of Re P and $\bar{\psi}\psi$ for the runs at $m_q = 0.0125a^{-1}$.

Many of these time histories show structure on long simulation time scales, and it is not clear at what point we have reached equilibrium. Our first run was at $6/g^2 = 5.60$ with $m_q = 0.025a^{-1}$. We have discarded the first 200 time units, and they are not shown in Figs. 1 and 2. The first run with $m_q = 0.0125a^{-1}$ was also at $6/g^2 = 5.60$ starting from an equilibrated lattice with the same coupling, but $m_q = 0.025a^{-1}$. The first 100 time units of this run were discarded, and are not shown in Figs. 3 and 4. All other runs were started from equilibrated lattices at neighboring couplings. All data from these runs are shown in Figs. 1–4. To make rough plots of the Polyakov loop and $\bar{\psi}\psi$ we have averaged the data shown in Figs. 1–4 omitting the first 100 time units in all but the short runs at $6/g^2 = 5.45$. For the latter we omitted only 25 time units. The error bars were estimated by blocking the data and calculating the apparent statistical error in the block averages. The block size was increased until the apparent error reached a plateau. The block sizes determined in this way ranged from 25 to 50 simula-

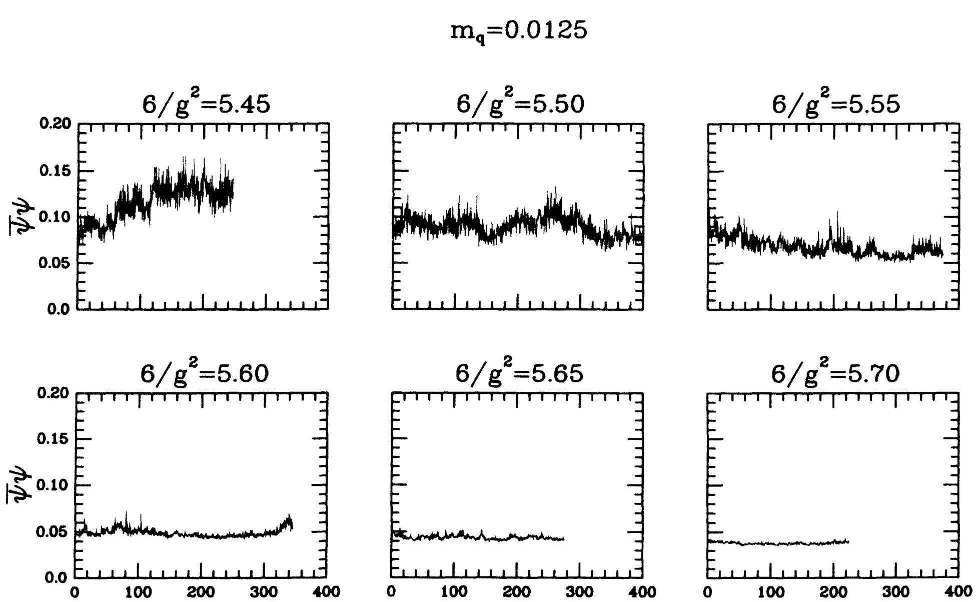

FIG. 4. Time histories of $\bar{\psi}\psi$ for $m_q = 0.0125$.

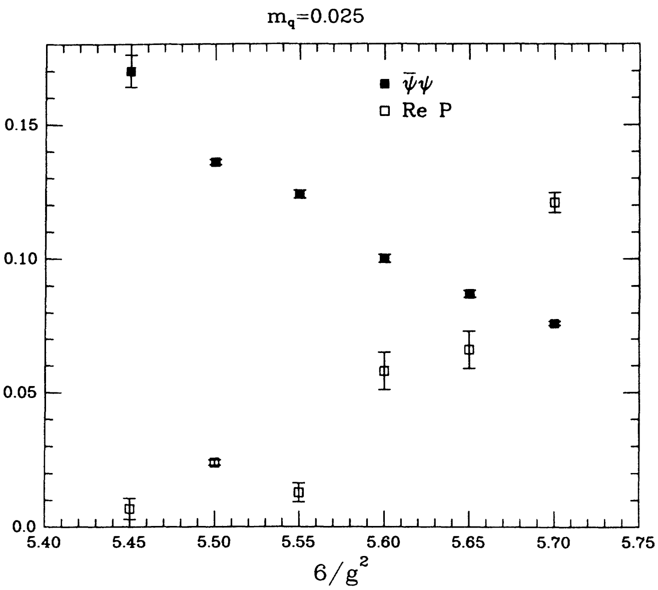

FIG. 5. The average value of $\bar{\psi}\psi$ and the real part of the Polyakov loop as a function of $6/g^2$ for $m_q = 0.025$.

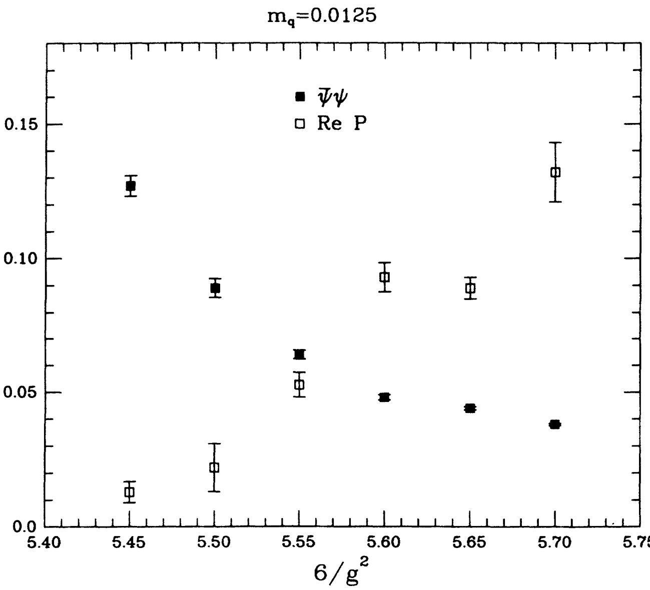

FIG. 6. The average value of $\bar{\psi}\psi$ and the real part of the Polyakov loop as a function of $6/g^2$ for $m_q = 0.0125$.

tion time units. This procedure produced the results in Fig. 5, which shows $\bar{\psi}\psi$ and the real part of the Polyakov loop as a function of $6/g^2$ for $m_q = 0.025a^{-1}$, and Fig. 6, which shows the same quantities for $m_q = 0.0125a^{-1}$.

III. CONCLUSIONS

These runs appear to show a rather broad crossover from low-temperature to high-temperature behavior. In the absence of results on larger spatial lattices and at smaller quark masses we cannot say whether this crossover would sharpen into a genuine phase transition as we increase the spatial size or decrease the quark mass. However, these results do provide an indication of where the crossover is. This is useful for guiding low-temperature simulations, where $6/g^2$ must be chosen small enough that the simulation is in the low-temperature regime. Also, when coupled with hadron mass estimates from low-temperature simulations at similar values of $6/g^2$ and m_q, these results could give an estimate of the physical transition or crossover temperature at $N_t = 8$. Finally, when results with larger spatial lattices and smaller quark masses become available these $12^3 \times 8$ results will be valuable in the analysis of finite-size effects and the effects of changing the quark mass.

ACKNOWLEDGMENTS

This work was supported by the Department of Energy under Contracts Nos. DE-AC02-84ER-40125, DE-FC05-85ER-250000, and DE-FG02-85ER-40213, and from the National Science Foundation under Grant No. PHY-86-14185. One of us (D.T.) was supported in part by the Alfred P. Sloan Foundation.

[1]The status as of September 1988 was reviewed by M. Fukugita, in *Lattice '88,* proceedings of the International Symposium, Batavia, Illinois, 1988, edited by A. S. Kronfeld and P. B. MacKenzie [Nucl. Phys. B (Proc. Suppl.) **9**, 291 (1989)]. Reports on recent work were presented at this symposium by S. Meyer, *ibid.*, p. 320; S. Gottlieb *et al.*, *ibid.*, p. 326; R. Gupta, *ibid.*, p. 473; and D. Sinclair, *ibid.*, p. 331.

[2]F. Karsch, J. B. Kogut, D. K. Sinclair, and H. W. Wyld, Phys. Lett. B **188**, 353 (1987); C. DeTar and J. B. Kogut, Phys. Rev. Lett. **59**, 399 (1987); Phys. Rev. D **36**, 2828 (1987); S. Gottlieb, W. Liu, D. Toussaint, R. L. Renken, and R. L. Sugar, *ibid.* **35**, 3972 (1987); Phys. Rev. Lett. **59**, 2247 (1987); **59**, 1881 (1987).

[3]S. Gottlieb, W. Liu, D. Toussaint, R. L. Renken, and R. L. Sugar, Phys. Rev. Lett. **59**, 1513 (1987); Phys. Rev. D **38**, 2245 (1988).

[4]H. Andersen, J. Chem. Phys. **72**, 2384 (1980); S. Duane, Nucl. Phys. **B257**, 652 (1985); S. Duane and J. Kogut, Phys. Rev. Lett. **55**, 2774 (1985).

[5]S. Gottlieb, W. Liu, D. Toussaint, R. L. Renken, and R. L. Sugar, Phys. Rev. D **35**, 2531 (1987).

[6]S. Gottlieb, W. Liu, D. Toussaint, R. L. Renken, and R. L. Sugar, Phys. Rev. D **36**, 3797 (1987).