Clear Evidence for a First-Order Chiral Transition in QCD

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We present evidence from numerical simulations for a first-order chiral-symmetry–restoration transition in QCD at finite temperature. The transition appears only for small quark masses. We use an exact algorithm to incorporate the dynamical quarks.

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Hadronic matter at high temperature and density is expected to undergo a transition to quark-gluon plasma. The present planned heavy-ion experiments will be able to investigate temperatures up to a few hundred megaelectronvolts. It is therefore very important to understand the nature of the transition and determine the transition temperature. The only quantitative tool available to address this nonperturbative phenomenon is the numerical simulation of lattice gauge theory. We have used the exact algorithm of Scalapino and Sugar[1] to study the phase diagram of QCD at small quark masses (m_q) using staggered fermions. In this paper we present clear evidence for a first-order chiral-symmetry–restoration transition at high temperature.

Simulations of pure gauge SU(3) show a strong first-order transition at a temperature $T_c \approx \Lambda_{\overline{\rm MS}}$ ($\overline{\rm MS}$ denotes the modified minimal-subtraction scheme).[2] At this transition the global $Z(3)$ symmetry of the theory is spontaneously broken. A nonzero expectation value of the Polyakov line $\langle L \rangle$ in the high-temperature deconfined phase implies a finite free energy for the quarks. A second-order parameter, the chiral condensate $\langle \bar{\chi}\chi \rangle$ measured in the quenched approximation, is also discontinuous at the transition. $\langle \bar{\chi}\chi \rangle$, when extrapolated to $m_q = 0$, changes from a nonzero value at low T to zero in the high-T phase.

Dynamical quarks act as external fields and explicitly break the $Z(3)$ symmetry. $\langle L \rangle$ is still a measure of the quark free energy but it is nonzero for all temperatures because of vacuum polarization. $\langle \bar{\chi}\chi \rangle$ remains a good order parameter to study chiral symmetry. The only theoretical understanding of the realization of chiral symmetry comes from a renormalization-group analysis of an effective-spin model in $4-\varepsilon$ dimensions.[3] The conclusion is that QCD has a first-order chiral-symmetry transition for $N_f \geq 3$ and at $m_q = 0$. For $T < T_c$, one expects $\langle \bar{\chi}\chi \rangle \neq 0$ when extrapolated to $m_q = 0$. For $T > T_c$ the chiral symmetry is restored, and consequently $\langle \bar{\chi}\chi \rangle \propto m_q$ for small m_q. This needs to be verified. Also, if, as in the pure gauge theory, there is a discontinuity in $\langle L \rangle$, then we expect to see interesting thermodynamical properties of the quark-gluon plasma[4] created in heavy-ion collisions.

The expected phase diagram for QCD is as follows: The confinement transition at $m_q = \infty$ extends to some finite m_q in the m_q-T phase plane, and similarly the chiral transition at $m_q = 0$ extends to some nonzero m_q. The questions to settle are whether these two transitions are connected and whether the chiral transition with the three physical light flavors is first order. The status of the chiral transition is not clear. We summarize the results for four flavors of staggered fermions obtained by approximate algorithms. The most detailed calculations are by Kogut and Sinclair[5] who find a rapid crossover for $m_q = 0.1$ and 0.5. Extrapolating the coupling at the center of the crossover to $m_q = 0$, they find that the transition coupling $6/g^2$ for $N_t = 6$ (4) is 5.01 ± 0.025 (≈ 4.9). Further, assuming that asymptotic scaling is valid, they estimate the transition temperature to be $T_c = (2.14 \pm 0.1)\Lambda_{\overline{\rm MS}}$. Similarly, Gavai[6] does not find evidence for a first-order transition. On the other hand, Fucito and Solomon[7] and Fukugita and Ukawa[8] claim that at these masses the transition is already first order. They find hysteresis in their runs, i.e., two metastable states. The chief criticism against the last two calculations is that the runs were not long enough for complete thermalization. The algorithm used to simulate fermions was different in each study and so the reason for conflict-

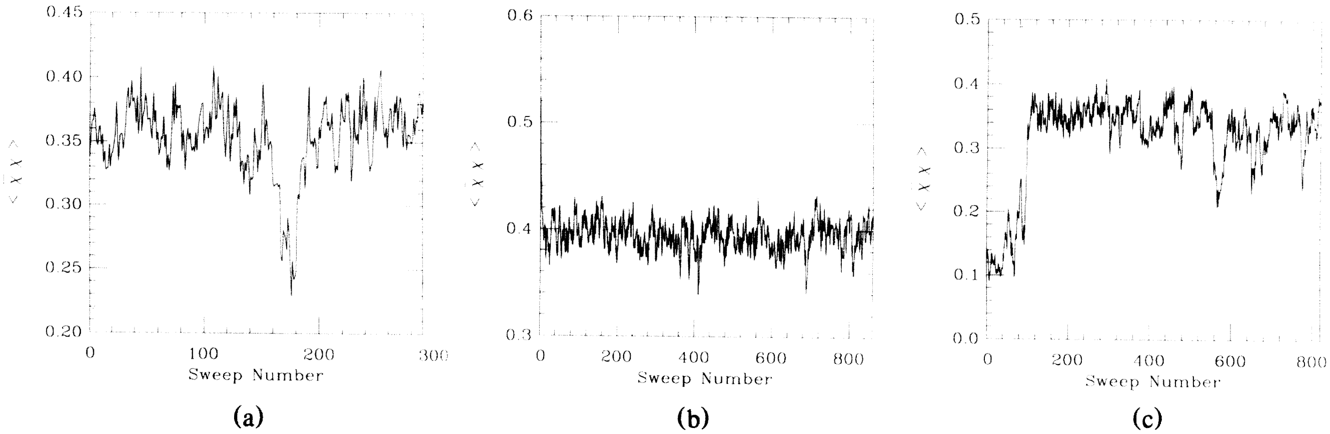

FIG. 1. Plot of $\langle\bar{\chi}\chi\rangle$ with $N_{CG}=60$ vs Monte Carlo sweeps at (a) $\beta=4.8$, $m_q=0.025$, (b) $\beta=4.9$, $m_q=0.10$, and (c) $\beta=4.9$, $m_q=0.05$.

ing results may also lie in the nature of the bias introduced by the approximations.

To address this issue we have made extensive runs using the exact algorithm. The largest lattice on which this can be done with reasonable statistics is $4\times4\times4\times4$. In exploring the small-m_q limit we find evidence for the chiral transition. Because of the small lattice size, and the fact that $N_s=N_t$, we cannot claim any quantitative results for T_c.[9] However, the clarity in the signal of the transition makes our qualitative result interesting. In particular, it resolves the above-mentioned dispute on the nature of the transition between the various approximate algorithms.

In the exact algorithm the ratio of determinants $R\equiv\det(1+M^{-1}\delta M)$ is calculated at each link update. Since we use staggered fermions (four flavors), the algorithm requires a calculation of a 6×6 block of M^{-1}. Because M^{-1} is calculated with the conjugate gradient (CG) iterative algorithm to some approximation, there can be a systematic bias. We discuss this later. In a Metropolis update, a link can be changed many times without our having to recalculate M^{-1}. The multihit algorithm we use is that described in detail by Gavai and Gocksch.[10] We use antiperiodic boundary conditions in all directions. We update each link with fifty hits and the acceptance is adjusted to $\approx 30\%$. In solving $Ax_{\text{even}}=M^\dagger M x_{\text{even}}=b$, we define the convergence by $C=\langle b-Ax\,|\,b-Ax\rangle/\langle x\,|\,x\rangle$, which depends on the number of CG iterations (N_{CG}).

In our data all the observables, $\langle\bar{\chi}\chi\rangle$, $\langle L\rangle$, Wilson loops, and R, are correlated. We use $\langle\bar{\chi}\chi\rangle$ to demonstrate the transition. At $6/g^2=4.8$, $m_q=0.025$, and with $N_{CG}=60$ there is no indication of a transition [Fig. 1(a)] in our small data sample. At $6/g^2=4.9$ and $m_q=0.1$, one sees only thermal fluctuations with $N_{CG}=60$ [Fig. 1(b)]. Similarly, for $m_q=0.05$ we do not see a two-state structure [Fig. 1(c)], but compared to $m_q=0.1$ the fluctuations are larger. The situation changes at $m_q=0.025$. For $N_{CG}=30$ [Fig. 2(a)], 60 [Fig. 2(b)], and 90 [Fig. 2(c)], we see metastability and a two-state behavior

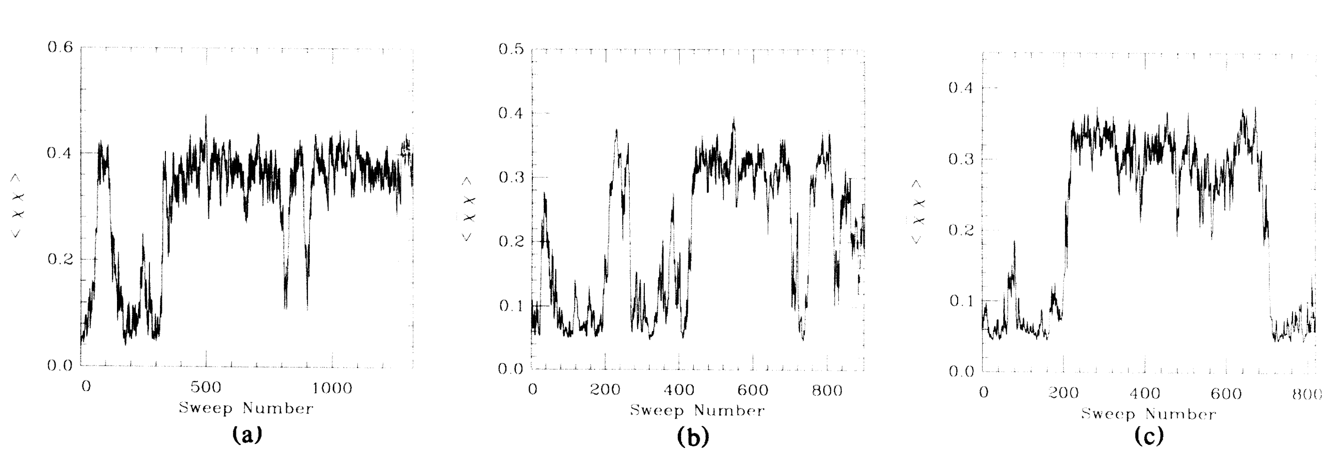

FIG. 2. Plot of $\langle\bar{\chi}\chi\rangle$ vs Monte Carlo sweeps at $\beta=4.9$, $m_q=0.025$ and (a) $N_{CG}=30$, (b) $N_{CG}=60$, and (c) $N_{CG}=90$. The two-state signal stands out in each case.

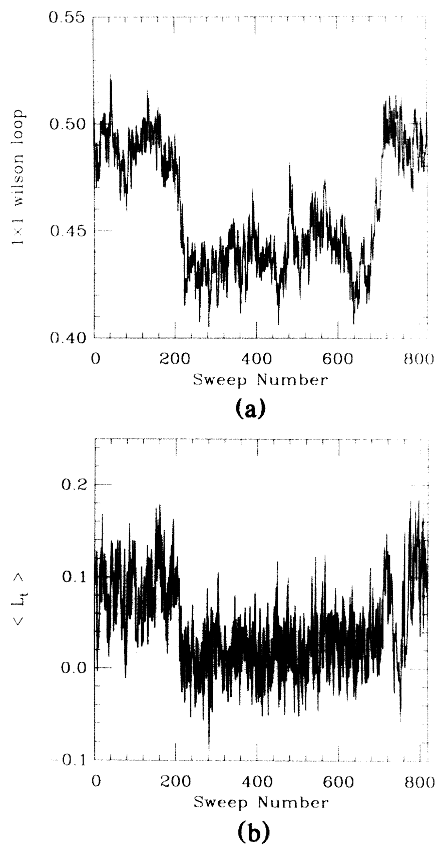

FIG. 3. Plot of (a) 1×1 loop, (b) $\langle L\rangle$ vs Monte Carlo sweeps at $\beta=4.9$, $m_q=0.025$, and $N_{CG}=90$. The correlation with $\langle\bar{\chi}\chi\rangle$ is striking for these observables.

characteristic of a first-order transition. To protect against inadequate thermalization, we run long enough to see flip flop between the states. In Figs. 3(a) and 3(b) we also show the data for 1×1 Wilson loop and $\langle L\rangle$ in one of the four directions (all four directions show similar behavior). There is a clear correlation between all observables. We regard this as evidence that at small m_q, QCD has a first-order transition with discontinuities in $\langle\bar{\chi}\chi\rangle$, $\langle L\rangle$, and Wilson loops. While the chiral and thermal transitions need not have been related, the data show that for $T>T_c$, the system is deconfined and chiral symmetry is restored.

To analyze the transition further we study $\langle\bar{\chi}\chi\rangle$ as a function of m_q. In the confined phase we estimate $\langle\bar{\chi}\chi\rangle-0.3\propto m_q$ from the data shown in Fig. 2. To study $\langle\bar{\chi}\chi\rangle$ in the high-temperature phase, we made runs with $N_{CG}=60$ at $6/g^2=4.95$ and $m_q=0.05$, 0.025, 0.02, and 0.015. We find a signal for the transition at the two heavier m_q, while the system is predominately in the deconfined phase at the two smaller m_q. Our estimates, 0.14(3), 0.07(3), 0.05(1), and 0.04(1), agree with the expected behavior $\langle\bar{\chi}\chi\rangle\propto m_q$.

We now present a preliminary analysis of the systematic biases in our simulation. Our implementation of the CG algorithm tends to underestimate the effects of the fermions, i.e., it tends to give too small a value for $S\equiv|\ln(R)|$. We have studied this by changing a single link and comparing the exact R with that calculated with a variety of CG sweeps. The exact R is obtained by calculation of the determinants, before and after a change in the link, by use of Gaussian elimination. At $m_q=0.1$, $N_{CG}=60$ suffices to give the exact answer, while for $N_{CG}=30$, S is underestimated by a few percent. For $m_q=0.025$, the algorithm requires $N_{CG}=90$ to get S good to a few percent, while for $N_{CG}=30$ the estimate of S is poor. These estimates remain valid when we make

TABLE I. Comparison of $\ln(\det R)$ for two configurations separated by twenty sweeps at $\beta=4.9$, $m_q=0.025$, and $N_{CG}=90$. Also given is the determinant and the mean convergence over twenty sweeps.

Config. No.	Accepted $\ln(\det R)$	True $\ln(\det R)$	$\ln(\det M)$	$\langle C\rangle\times10^7$
1			110.3	1.3
2	-2.9	-2.9	107.4	1.0
3	-0.5	-0.3	107.0	1.4
4	-40.1	-36.6	70.4	0.9
5	29.6	30.9	101.4	3.9
6	5.1	5.1	106.5	0.9
7	-4.5	-4.5	102.0	0.9
8	6.1	6.1	108.1	1.1
9	-24.8	-24.3	83.7	3.6
10	4.8	5.5	89.3	2.6
11	-53.4	-45.3	43.9	20.
12	-1.1	6.4	50.4	26.
13	-27.8	-17.2	33.1	26.
14	8.4	14.8	47.9	26.
15	-11.1	1.6	49.6	26.
16	-8.4	-2.3	47.2	26.
17	7.6	12.2	59.4	26.
18	-27.4	-21.2	38.1	25.
19	10.3	24.4	62.6	26.
20	-22.0	-18.4	44.1	24.
21	-3.4	1.4	45.6	26.
22	-2.9	4.5	50.1	26.
23	-15.6	-7.0	43.1	26.
24	24.7	29.8	72.9	26.
25	-26.9	-20.6	52.2	24.
26	-13.7	-2.1	50.1	26.
27	0.7	9.4	59.5	24.
28	-4.7	-2.2	57.3	24.
29	-5.3	4.7	62.1	23.
30	-12.1	-7.3	54.7	25.
31	-11.3	-3.8	50.9	25.
32	-30.2	-19.2	31.6	26.
33	8.6	19.0	50.6	26.
34	-6.2	4.9	55.6	26.
35	5.4	9.8	65.4	23.
36	44.0	44.4	109.8	6.7
37	-3.1	-3.1	106.7	0.9
38	-13.7	-13.7	92.9	1.0
39	-9.9	-9.5	83.3	1.5
40	19.8	19.9	103.3	1.7
41	-1.4	-1.9	101.4	3.0

multiple hits on the same link.

To study if there is an accumulation of the bias, we compare the product of the accepted determinant ratios ($A \equiv \ln R_{\rm acc}$) with the exact answer (T). The data for $m_q = 0.025$ and $N_{\rm CG} = 90$ are shown in Table I, together with $\ln(\det M)$ and $\langle C \rangle$. In the high-temperature phase (1–10 and 36–41) one finds $A \le T$, with only small deviations from equality. On the other hand, the confined phase (11–35) has A significantly less than, though correlated with, T. This phase also shows a marked deterioration in $\langle C \rangle$, suggesting that M has small eigenvalues not present in the high-temperature phase. The difference between A and T is large, but it has been accumulated over $\approx 20 \times 0.3 \times 50 \times 4 \times 4^4$ link changes, and so corresponds to a tiny bias in R for each change.

The disagreement between A and T gets progressively worse with decreasing $N_{\rm CG}$, but C is consistently a factor of ≈ 20 smaller in the high-temperature phase. Conversely, the bias decreases as m_q increases. It is unobservable for $m_q = 0.1$, $N_{\rm CG} = 60$.

All this suggests that $C \le 10^{-7}$ is necessary to avoid a bias at $6/g^2 = 4.9$, $m_q = 0.025$. Our best data do not quite meet this requirement, but the presence of the transition for all values of $N_{\rm CG}$ makes it very likely that the transition would remain for $N_{\rm CG} = \infty$.

To conclude, we show that there does exist a first-order chiral-thermal transition at small m_q. Its uncertainty in previous calculations is due to its abrupt appearance at a smaller m_q.

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