Return of the Finite-Temperature Phase Transition in the Chiral Limit of Lattice QCD

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Lattice QCD with four flavors of light dynamical quarks is simulated on a $10^3 \times 6$ lattice in order to study the finite-temperature transition in the chiral limit. The mass used, $m=0.025$ (in lattice units), is half the smallest value previously used on this size lattice. We find evidence for a finite-temperature phase transition which is absent for intermediate masses. The time evolution of the system shows both long correlation times characteristic of a nearby critical point and abrupt changes.

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The finite-temperature behavior of QCD is of interest not only because it gives insight into the nonperturbative dynamics of the theory, but also because a heavy-ion collider should make the transition between hadronic matter and the quark-gluon plasma observable in the laboratory. Such a transition certainly occurred in the early Universe and may have influenced the evolution of its large-scale structure.

Computer simulations of lattice QCD have been used to study this phenomenon. In the absence of dynamical quarks a strong first-order deconfining transition at a finite temperature was observed some time ago.[1] This phase transition survives the addition of massive dynamical quarks[2] but as the mass is decreased the simulations show that the transition softens and probably disappears.[3] However, for massless quarks one expects a chiral-symmetry–restoring phase transition. If this transition is strong enough that its influence extends to small but finite quark mass, then it should be interesting and accessible experimentally. Such would be the case if one had a line of phase transitions (probably first order) extending from zero to finite quark mass and terminating in a critical point. (On theoretical grounds one would expect this transition to be first order for sufficiently small quark mass.[4]) The study presented here supports this optimistic scenario.

The computer-simulation technique employed in this study is a slightly improved version of the hybrid algorithm[5] we have used in earlier studies of the thermodynamics of QCD at intermediate values of the quark mass.[3] One begins with the molecular-dynamics Lagrangean,

$$L=\frac{1}{2}\sum_{\substack{u\\ \text{links } l}} \dot{U}_\mu^\dagger(l)\hat{P}\dot{U}_\mu(l)+\sum_{\substack{mn\\ \text{even sites}}} \dot{\psi}_m^\dagger[(-\boldsymbol{D}+m)(\boldsymbol{D}+m)]_{mn}\dot{\psi}_n-\omega^2\sum_{\substack{n\\ \text{even sites}}}\psi_n^\dagger\psi_n-\beta\sum_{\square}\mathrm{tr}[UUUU+\mathrm{H.c.}], \tag{1}$$

where $\hat{P}=\mathrm{diag}(1,1,0)$ in color space, $\beta=6/g^2$, and the time derivatives refer, essentially, to the computer-simulation time. The ψ variables, which reside on even lattice sites, are commuting pseudofermion fields. The factor of $(-\boldsymbol{D}+m)(\boldsymbol{D}+m)$ in the kinetic-energy term for the ψ field ensures that the correct fermion determinant is generated when ψ and its conjugate momentum are integrated out of the system's canonical partition function. Since we use staggered fermions on the lattice, the lattice determinant gives rise to four flavors of quarks in the theory's continuum limit. In a microcanonical (molecular-dynamics) simulation of Eq. (1) the deterministic equations of motion would be implemented. In the hybrid algorithm one touches the isolated physical system of Eq. (1) to a heat bath at the desired "temperature" (which we choose to be 1) from time to time during the molecular-dynamics simulation. This refreshment procedure ensures ergodicity and speeds the convergence rate of the algorithm, so that time averages of observables are identical to ensemble averages of interest in thermodynamics and field theory. In the numerical implementation of this procedure one chooses a discrete time step dt. This approximation induces a calculable systematic error in the equilibrium distribution field configurations. These effects can be absorbed into shifts of the bare parameters, β and mass, of the Lagrangean Eq. (1) provided dt is small enough.[5,6] At small fermion masses such as the $m=0.025$ of this study, even with the small dt chosen, we expect systematic errors larger than our statistical errors. However, because they can be absorbed into β and m, they

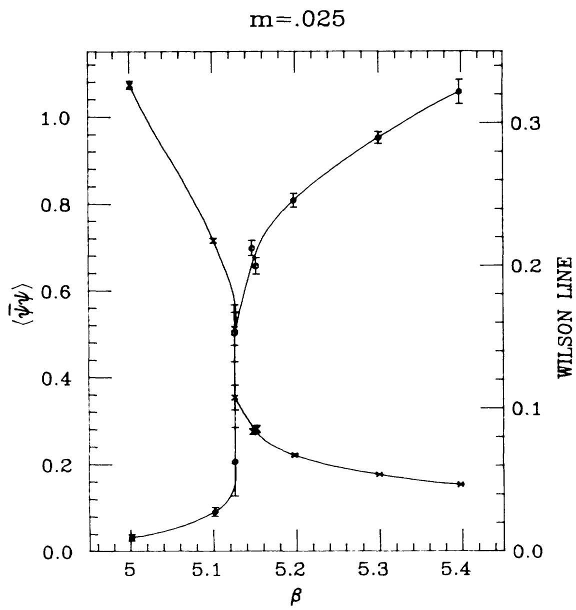

FIG. 1. Wilson line (crosses) and $\langle\bar{\psi}\psi\rangle$ (circles) as functions of $\beta=6/g^2$.

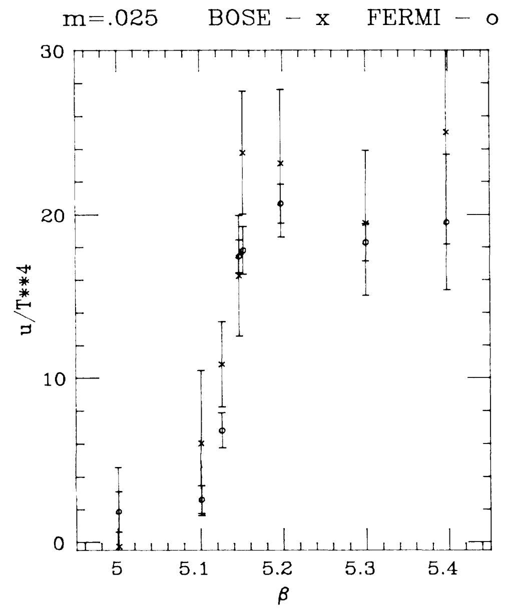

FIG. 2. Gluon and fermion energy densities u as functions of $\beta=6/g^2$.

should not affect our qualitative predictions. The numerical integration of the equations of motion and the heat-bath step are accurate to $O(dt^4)$ at each step.

Runs were performed at (input) β values of 5.4, 5.3, 5.2, 5.1, 5.15, 5.125, 5.1, and 5.0 using $dt=0.01$ and refreshing every 100 sweeps. (Some runs were also done at $\beta=5.4$ and 5.3 with $dt=0.02$.) The number of sweeps at each β varied from 30000 far from the transition to 166000 for $\beta=5.125$, which is very close to the observed transition. We discarded a minimum of 10000 sweeps at each β for equilibration. The statistical errors were corrected for the observed time correlations.

We now present the results of these extensive runs. In Figs. 1 and 2 we show the equilibrium measurements of the chiral order parameter $\langle\bar{\psi}\psi\rangle$, the Wilson line, and the gluon and fermion energy densities. Changing β from 5.15 to 5.1 results in an abrupt change of $\langle\bar{\psi}\psi\rangle$ from ~ 0.3 at $\beta=5.15$ in the quark-gluon phase to ~ 0.7 at $\beta=5.1$ in the hadronic-matter phase while the Wilson line falls from ~ 0.2 to ~ 0. The energy densities shown in Fig. 2 change as abruptly over the same region. These figures should be compared with the analogous ones corresponding to the quark mass $m=0.050$ in Ref. 3. Clearly, decreasing the fermion mass has made the transition region between the hadronic and the quark-gluon phases noticeably narrower and suggests a first-order transition for masses below $m=0.025$ on $10^3\times 6$ lattices. The rapid change in the energy densities is an encouraging result for the planners of heavy-ion facilities—the bulk thermodynamic changes at the transition are very pronounced. The exact nature of the transition is, however, more difficult to ascertain. Is it second order, fluctuation-induced first order, or strongly first order? An indication that the value $m=0.025$ lies close to a critical point comes from a calculation of the correlation times for the Wilson line and $\langle\bar{\psi}\psi\rangle$ at β values near the transition. Table I shows the time autocorrelation lengths and a substantial peak at the transition is apparent. This suggests critical slowing down which would be characteristic of a nearby critical point. Finally, in Figs. 3 and 4 we show the time evolution of $\langle\bar{\psi}\psi\rangle$ at $\beta=5.125$ and 5.1. The starting configuration in Fig. 3 was in the plasma phase, equilibrated at a β value very close to 5.125. The evolution of the system shows signs of metastability with coexisting plasma and hadronic phases suggesting a (weak) first-order transition. However, we also notice large-scale fluctuations with long

TABLE I. "Time" autocorrelation lengths. Note that since the time correlation function is not a simple exponential these values are somewhat subjective. Near the transition they clearly underestimate the long-time correlations of the system (see Fig. 3).

β	$\tau_{\langle\bar{\psi}\psi\rangle}$	$\tau_{\text{Wilson line}}$
5.398 ± 0.002	0.7	2.1
5.300 ± 0.002	0.9	1.2
5.198 ± 0.002	1.5	1.7
5.152 ± 0.001	7.5	2.5
5.147 ± 0.002	5.0	2.4
5.126 ± 0.001	>8.6	>6.5
5.101 ± 0.001	0.8	1.4
5.001 ± 0.001	1.0	0.3

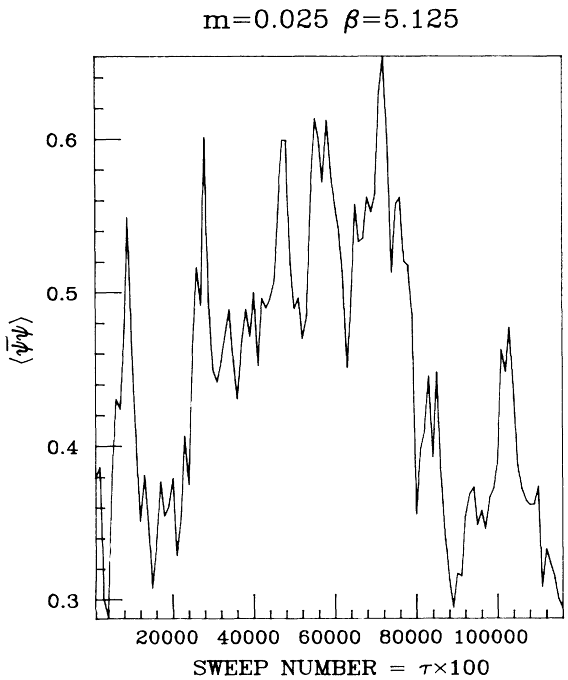

FIG. 3. Time evolution of $\langle\bar{\psi}\psi\rangle$ at $\beta=5.125$.

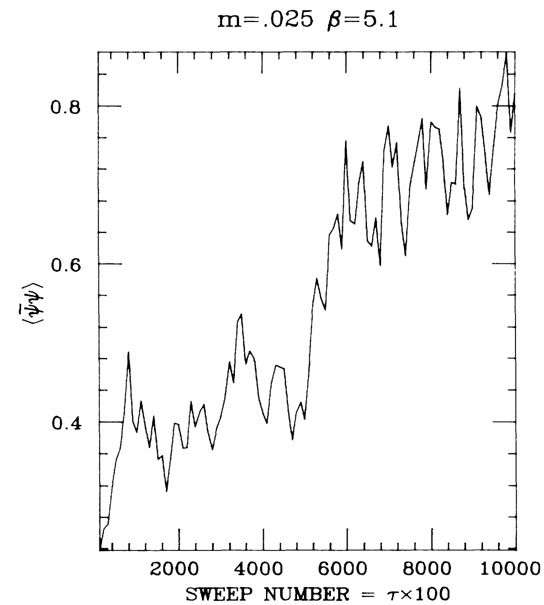

FIG. 4. First 10000 sweeps of time evolution of $\langle\bar{\psi}\psi\rangle$ at $\beta=5.1$.

time constants ~10000–20000 sweeps (with $dt=0.01$), a characteristic of a system near a critical point. In Fig. 4 we see an abrupt jump in $\langle\bar{\psi}\psi\rangle$ in the time evolution at $\beta=5.1$, also suggestive of a first-order transition, but no metastability is observed (in 90000 sweeps).

This work demonstrates that with the algorithms and computing power currently available, we are inching toward a quantitative understanding of the chiral limit of QCD. Past studies of the thermodynamics of QCD at large fermion masses showed a strongly first-order hadronic-matter–quark-gluon-plasma transition. At intermediate values of the quark mass on $10^3\times 6$ lattices the transition is softened and is probably no longer a phase transition. However, as m is decreased below 0.025 we have found evidence for a short line of first-order transitions extending from the $m=0.0$ chiral limit. Critical slowing down suggests that there is a critical point at the end of this line near $m=0.025$ and $\beta=5.125$. Perhaps of most relevance to the experimental physics community is the fact that the transition occurs at an accessible temperature and with large changes in observable internal energies. As discussed in Ref. 3, if we apply asymptotic-freedom scaling laws to our data and extrapolate to $m=0.0$, the chiral transition should occur at

$$T_c=(2.14\pm 0.10)\Lambda_{\overline{\rm MS}},$$

where $\overline{\rm MS}$ denotes the modified minimal-subtraction scheme. Our new data at $m=0.025$ showing a phase transition at $\beta=5.125\pm 0.025$ are consistent with this prediction. The energy densities in the quark-gluon phase saturate the Stefan-Boltzmann free-field values just above the transition.

We are engaged in several projects to improve our understanding of the issues discussed in this Letter. In order to search for metastability we are simulating $8^3\times 4$ lattices at even smaller masses, $m=0.0125$ and $m=0.025$, in addition to $m=0.0375$. Preliminary results are encouraging and we believe that there are coexisting states in these cases. This result would complement a recent exact calculation on a very small (4^4) lattice.[7] In addition, our runs on the $10^3\times 6$ lattice continue.

These $10^3\times 6$ lattice simulations were performed by use of over 5000 hours of central processing unit time on an ST-100 array processor. This computer averaged 50 Mflops (about $\frac{2}{3}$ the performance we obtained on a Cray X-MP/24) during these simulations.

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