On the Existence of a Phase Transition for QCD with Three Light Quarks

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We report full QCD simulations on a $16^3\times4$ lattice. For two degenerate flavors no finite-temperature phase transition is found for quark masses of $ma=0.01$ and 0.025, where a is the lattice spacing, while for three degenerate flavors a first-order transition is easily seen for $ma=0.025$. Nature, with nearly massless up and down quarks and one heavier strange quark, lies between these two cases. For $m_{u,d}a=0.025$ and $m_sa=0.1$ we find that $m_K/m_\rho=0.46(1)$ and that no transition occurs, calling into question the existence of a QCD phase transition.

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One of the most dramatic predictions of quantum chromodynamics (QCD) is the creation of a plasma of quarks and gluons when the QCD vacuum is heated to a temperature of a few hundred MeV. This significant temperature dependence of the QCD vacuum may well have observable consequences for heavy-ion collisions and the evolution of the early Universe. Although the quark-gluon plasma and the low-temperature QCD vacuum are very different in structure and are usually pictured as being separated from one another by a deconfining (or chiral-symmetry restoring) phase transition, no formal arguments require such a transition to exist for finite quark mass, and a number of QCD simulations (on coarse lattices) show that no transition occurs for moderately massive quarks.[1] It is an open question whether real-world QCD with nearly massless up and down quarks and a rather light strange quark has a finite-temperature transition. We report here that on unphysically coarse lattices Monte Carlo calculations with nearly realistic quark masses show no such transition.

Under the assumption that at low temperature QCD both confines and spontaneously breaks chiral symmetry, theoretical arguments constrain the QCD phase transition for infinite and zero quark mass. Proofs on the lattice that at high temperature the Z_3 symmetry of pure gauge QCD breaks spontaneously, signaling deconfinement,[2] and the chiral symmetry of QCD with massless quarks is restored,[3] show that the high-temperature systems realize exact symmetries differently than assumed at low temperature, requiring the occurrence of a phase transition. Furthermore, these symmetries imply that the pure SU(3) gauge transition should be first order,[4] and that the zero-mass transition, although possibly second order for two massless flavors, should be first order for the number of flavors (N_f) three or greater.[5]

So far, these expectations have been borne out by lattice-gauge-theory calculations. In particular, four-flavor simulations with four and six temporal lattice spacings (N_t) show a first-order transition when the quark mass is either sufficiently large or sufficiently small.[1] The four-flavor calculations also illustrate an important effect of massive quarks—they can eliminate the transition. Because the relevant symmetries are explicitly broken by quarks with finite mass, symmetry arguments no longer imply the existence of a transition, and indeed for four flavors of intermediate mass the low-temperature QCD vacuum evolves continuously into the quark-gluon plasma with increasing temperature.[1]

As a step towards determining whether real-world QCD has a finite-temperature transition, we have performed a series of Monte Carlo simulations on a $16^3\times4$ lattice with two and three flavors of light quarks. In Fig. 1 we summarize our results by charting the values of two masses—those of the strange quark and the degenerate up and down quarks—for which a transition occurs for some temperature. Figure 1 is in part conjectural; it represents our proposal for the simplest such diagram consistent with established results. The upper border of the diagram corresponds to two degenerate flavors. Our calculations suggest that two massless flavors have a

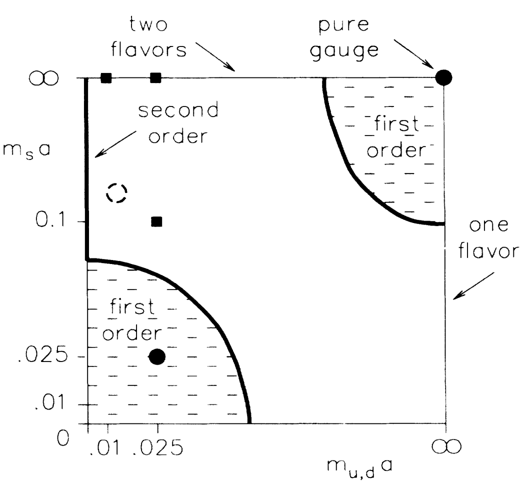

FIG. 1. Presence and absence of the finite-temperature QCD phase transition as a function of $m_{u,d}a$ and m_sa. Mass values for which the transition is and is not seen on a $16^3\times4$ lattice are denoted respectively by solid circles and squares. The physical point, indicated roughly by the dashed circle, lies in the region of no transition.

second-order transition that is washed out by any finite mass. In contrast, three light flavors show a first-order transition that is absent for larger mass. We therefore expect that for light up and down quarks there is a strange-quark mass below which the transition is first order and above which no transition occurs. Where does the mass of the physical strange quark lie? For $N_t=4$ we conclude that the physical strange-quark mass is close to, but above, the mass at which the transition disappears. We emphasize, however, that because $N_t=4$ is far from the continuum limit (which requires $N_t \geq 10$ for pure gauge QCD), significant changes are expected to occur in the physical $a \to 0$ limit.

The calculations reported here used the dynamical fermion R algorithm of Gottlieb *et al.*,[6] and ran for about six months on the 256-node Columbia machine, a 16×16 grid of fast-array processors, at a sustained speed of 6.4 Gflops.[7] The algorithm evolves the gauge fields with respect to the action

$$S=\tfrac{1}{3}\beta\sum_{\mathcal{P}}\mathrm{Re\,tr}U_{\mathcal{P}}-\tfrac{1}{4}N_{u,d}\ln\det(D+m_{u,d}a)$$
$$-\tfrac{1}{4}N_s\ln\det(D+m_s a)\,,$$

where $U_{\mathcal{P}}$ is the product of the link matrices forming the boundary of the elementary plaquette $\mathcal{P}$. Because of fermion doubling the massless Kogut-Susskind Dirac operator, given by

$$(D\phi)_n=\tfrac{1}{2}\sum_{\mu}\eta_{n,\mu}(U^{\dagger}_{n,\mu}\phi_{n+\mu}-U_{n-\mu,\mu}\phi_{n-\mu})\,,$$

where $U_{n,\mu}$ and $\eta_{n,\mu}$ are the link matrices and Kogut-Susskind sign factors associated with the link at site n with direction μ, corresponds to four flavors of quarks. The factors of $\frac{1}{4}$ in the action "fractionalize" the doubled fermions so that setting $N_{u,d}=2$ and $N_s=1$ yields two degenerate flavors of mass $m_{u,d}$ and one of mass m_s. Although this action reproduces continuum N_f-flavor QCD order by order in perturbation theory, the fractional fermion determinant cannot be obtained by integrating quarks out of a theory with local interactions. Thus these calculations can be interpreted as describing four-dimensional classical statistical mechanics with a local Hamiltonian or three-dimensional quantum statistical mechanics with a well-defined transfer matrix only in the $a\to 0$ limit. The algorithm introduces errors of $O(\Delta\tau^2)$—we use a step size (normalized as in Ref. 6) of $\Delta\tau=0.0078$ for the $N_f=2$, $ma=0.01$ runs, and $\Delta\tau=0.01$ for the others. We use a conjugate gradient stopping condition of $(r^2/V)^{1/2}=8\times 10^{-5}$, in the notation of Ref. 8. In all cases the molecular-dynamics "momenta" are randomized after trajectories of $\frac{1}{2}$ units of time; measurements are performed on the gauge configurations obtained after each trajectory. We denote by $\bar\psi\psi$ the quantity $\sum_{l,n}h_l^*[(D+m)^{-1}]_{l,n}h_n$ averaged over three sets of h_n's for each gauge configuration, where for each site n, h_n is an independent complex three-vector of Gaussian random numbers normalized such that $\langle\sum_n|h_n|^2\rangle=1$.

Evidence that the transition is first order for three flavors with $ma=0.025$ is shown in Fig. 2. Two independent evolutions of $\bar\psi\psi$ as a function of molecular-dynamics time are shown for $\beta=5.132$. The run begun with an ordered lattice ($U_{n,\mu}=1$, initially) displays approximate chiral symmetry. The disordered start ($U_{n,\mu}$'s chosen randomly) remained in the phase of broken chiral symmetry for about 2500 units of time, tunneled to the symmetric phase, and then appears to have tunneled back at the end of the run. We also have ordered and disordered runs at $\beta=5.13$ where the chirally symmetric phase tunnels after 1500 units of time and at $\beta=5.135$ where the disordered start gradually evolves into the symmetric phase over a period of nearly 1500 units of time. For $\beta=5.13$ and 5.132 one sees a two-state signal with $\langle\bar\psi\psi\rangle\approx 0.24$ for the asymmetric phase and $\langle\bar\psi\psi\rangle\approx 0.13$ for the other. For $\beta=5.135$ only the symmetric phase can be identified. These results agree with earlier work on $4^3\times 4$ and $8^3\times 4$ lattices.[9,10]

Calculations with $N_f=2$ and the same mass of $ma=0.025$, however, showed no evidence for a first-order transition—no metastability or two-state signal was observed. We then lowered the mass to $ma=0.01$. Ordered and disordered starts at $\beta=5.25$ both relaxed in less than 100 time units into a chirally asymmetric state while similar starts for $\beta=5.275$ each relaxed into the symmetric phase in less than 200 time units. We then performed the long run at $\beta=5.265$ shown in Fig. 3. Large fluctuations and long correlation times are evident but again no two-state signal is seen. Figure 4 shows histograms of these runs. The single-peaked structure of each of the runs suggests that there is no transition for these values of β, and the overlap of the histograms provides evidence that a transition at an intermediate value of β has not been overlooked. Previous calculations for $ma\leq 0.05$ are in conflict: Some on $8^3\times 4$ and smaller lattices are claimed to show a transition,[10,11] while other, similar calculations[12] and a recent, careful study of

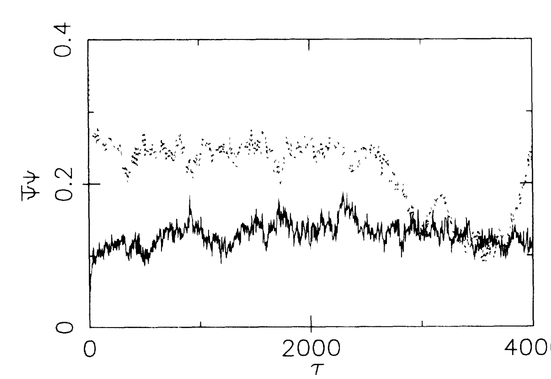

FIG. 2. Monte Carlo evolutions of $\bar\psi\psi$ for $N_f=3$, $ma=0.025$, and $\beta=5.132$. The behavior of the ordered start (solid) and disordered start (dotted) evolutions signals a first-order transition.

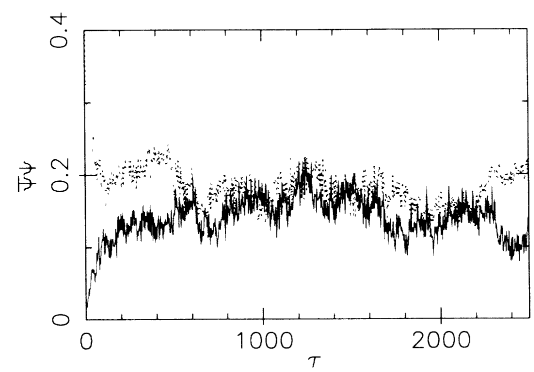

FIG. 3. Evolutions analogous to Fig. 2 for $N_f = 2$, $ma = 0.01$, and $\beta = 5.265$. The two starts mix together without clear tunneling events, indicating that no transition occurs.

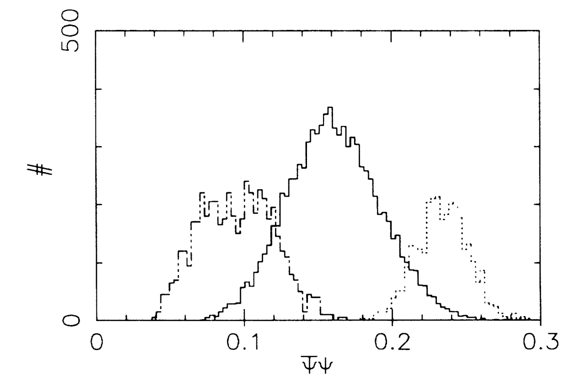

FIG. 4. Overlapping histograms show that for two flavors of $ma = 0.01$ $\bar{\psi}\psi$ evolves continuously with β without developing a two-peaked structure. From left to right, the histograms correspond to $\beta = 5.275$, 5.265, and 5.25. Counts are in units of trajectories, and have been scaled up by factors of 5 and 3 for $\beta = 5.275$ and 5.25, respectively. The first 500 trajectories of each run were discarded.

$ma = 0.025$ on lattices as large as $12^3 \times 4$ (Ref. 13) do not. We argue that our $16^3 \times 4$ results should resolve the question, and conclude that a transition does not occur for two flavors even with a mass as low as $ma = 0.01$.

Next let us consider simulations with two light flavors of $m_{u,d}a = 0.025$ and a strange quark with several values of a heavier mass, $m_s a$. Sets of runs for various values of β performed at $m_s a = 0.05$ and 0.5 totaled 3800 and 7200 units of time, respectively. Although not definitive, they strongly suggest that the smaller mass has a transition, while the larger does not. We concentrated our efforts on the case $m_s a = 0.1$ with the results shown by the evolution in Fig. 5. Although this run appeared to relax quickly to the two metastable states seen for $N_f = 3$ in Fig. 2, after 1000 units of time its character changed and the remainder of the evolution shows no two-state signal and gives an average for $\langle \bar{\psi}_{u,d} \psi_{u,d} \rangle$ midway between the values found for the ordered and disordered states. Thus, even for this light strange-quark mass, the system resembles $N_f = 2$ and has no transition, a result that conflicts with earlier reports of a clear transition on an $8^3 \times 4$ lattice[14] and less compelling evidence for a transition on a $12^3 \times 4$ lattice.[15]

In order to provide a physical interpretation for these quark mass values we have calculated hadron masses in a separate $T = 0$ simulation on a $16^3 \times 24$ lattice with $\beta = 5.171$, $m_{u,d}a = 0.025$, and $m_s a = 0.1$. We began with an ordered start, discarded the first 450 time units, and collected an additional 600 units of time, computing hadron propagators after every $\frac{1}{2}$ time unit trajectory. Except for the use of an extended, Coulomb-gauge-fixed source, our methods are the same as in Ref. 8. The results, shown in Table I, suggest that (a) the choice $\beta = 5.171$ is far from the continuum; the two kaons, for example, should be degenerate, but differ in mass by a factor of 2. (b) Using the calculation to establish a physical length scale is difficult given the large discrepancy between the mass ratio $m_N/m_\rho = 1.5(1)$ obtained from Table I and its physical value of 1.22. (c) The ratio $m_K/m_\rho = 0.46(1)$ is smaller than its physical value of 0.64, suggesting that the three-flavor, first-order transition disappears with increasing m_s before the strange quark reaches its physical mass. (d) Of possible concern is the relatively large value of the pion mass shown in Table I. However, in similar $N_t = 4$, four-flavor simulations $ma = 0.025$ lies well within the chiral limit,[16] indicating that the structure of the transition and m_K/m_ρ should be nearly independent of $m_{u,d}$.

Dynamical quarks strongly affect QCD thermodynamics. The results presented here suggest that even the existence of the QCD phase transition depends on the precise value of the strange-quark mass. These results support the picture shown in Fig. 1 in which we identify regions of $m_{u,d}$ and m_s for which a transition occurs. Our calculations suggest that for $N_t = 4$ the point corresponding to physical values of the quark masses lies outside the

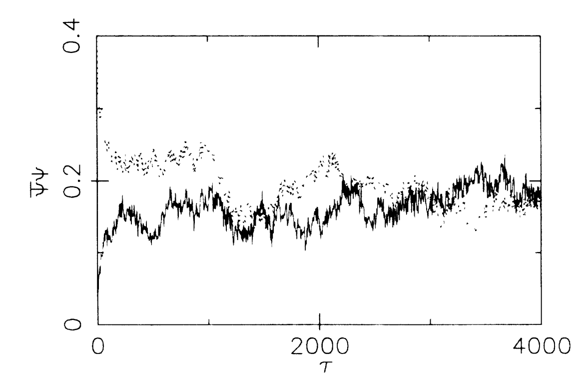

FIG. 5. Evolutions analogous to Fig. 2 for three quarks with nearly physical masses show no transition. The two flavors for which $\bar{\psi}\psi$ is plotted have $m_{u,d}a = 0.025$, the third has $m_s a = 0.1$, and $\beta = 5.171$.

TABLE I. A summary of the masses, measured in lattice units, determined from our $16^3\times 24$, $\beta=5.171$ simulation. We minimize, display in the table, and determine the errors from χ^2, using the full covariance matrix. The fits extend between r_{min} and 12 units of lattice separation. The pairs (π,π_2), (K,K_2), and (ρ,ρ_2) should each become components of degenerate flavor multiplets as $a\to 0$. Chiral symmetry is partially broken by the lattice and only protects the masses of the lighter π and K.

	mass$\times a$	χ^2	r_{min}
π	0.4117(4)	4	8
π_2	1.09(8)	5	4
K	0.6367(2)	6	7
K_2	1.34(3)	7	4
ρ	1.39(3)	16	4
ρ_2	1.41(7)	9	4
N	2.07(12)	12	3

first-order region, and raises the question whether this situation persists in the continuum limit, in which case real-world QCD would not have a finite-temperature phase transition.

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