

Finite-Size Test for the Finite-Temperature Chiral Phase Transition in Lattice QCD

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A finite-size test was carried out for the finite-temperature chiral phase transition in QCD for flavor number $N_f=4$ and 2 on a lattice with four time slices using the Kogut-Susskind quark action at quark mass of 0.025 in lattice units. All the evidence supports a first-order transition for $N_f=4$. For $N_f=2$, however, the data on spatial lattices up to 12^3 fail to yield convincing finite-size signatures for a first-order transition at this quark mass.

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A large amount of effort and computing time have been invested in order to elucidate the nature of the finite-temperature phase transition of quantum chromodynamics in the presence of dynamical quarks.^{1,2} The picture that emerged was that the phase transition first weakens from the pure-gauge limit toward intermediate quark masses, but reappears as a first-order chiral phase transition at a small quark mass for flavor number $N_f=4$ (Ref. 1) and 2 (Ref. 2). This conclusion was based on studies^{1,2} made mostly before 1987,³ and the evidence taken to indicate a first-order transition seems insufficient by today's standards. This is illuminated by the recent issue concerning the order of the pure-gauge deconfining phase transition;⁴ while we had thought the evidence obtained in early studies fairly clear, it turned out to require significantly more elaborate investigations⁵ to establish the first-order nature of the transition.

The past evidence for a first-order chiral transition in full QCD is mostly based on the detection of metastability and of associated two-state signals. On the lattices of relatively small spatial sizes that have been used, however, the separation of two states is not quite obvious. The problem is that the time of staying in one phase is comparable to the transition time between different phases, which would prohibit an unambiguous interpretation for a first-order transition. Doubt has also been cast from finite-size studies⁶ of the chiral transition at a moderately small quark mass of $m_q=0.1$ (in lattice units), which indicate that the first-order signatures might disappear in the thermodynamic limit.

In this situation we feel it necessary to reexamine to what extent a first-order chiral transition can be established for finite-temperature QCD with light dynamical quarks for $N_f=2$ and 4. Our strategy for this purpose is the use of finite-size scaling of susceptibilities.⁷ This method is very powerful in distinguishing a first- from a higher-order phase transition as we have shown for the pure-gauge deconfining transition.⁸ Its power is demonstrated even for the quite subtle case of the two-dimensional Potts model.⁹ A serious limitation for applying this test to full QCD is the computing power re-

quired to obtain data with sufficient accuracy. The simulation is at least a few thousand times more time consuming than the pure-gauge case, and hence we have to be content with relatively small spatial sizes of the lattice, ranging from $N_s^3=4^3$ to 12^3 , with the temporal size fixed at $N_t=4$. However, we increased the statistics by an order of magnitude over the previous studies^{1,2} at small quark masses.

The full QCD system we study is defined by the partition function

$$Z = \int \prod dU_l \prod d\chi_n d\bar{\chi}_n \exp(S_g + S_q), \quad (1)$$

with S_g the standard single-plaquette gauge action, and the Kogut-Susskind form taken for the quark action $S_q = \sum \bar{\chi}_n D_{n,n'} \chi_{n'}$, where

$$D_{n,n'} = m_q + \frac{1}{2} \sum \eta_{n,\mu} (\delta_{n,n'+\hat{\mu}} U_{n\mu} - \delta_{n,n'+\hat{\mu}} U_{n'\mu}^\dagger), \quad (2)$$

with n_{μ} the sign factor, which corresponds to $N_f=4$ in the continuum limit. For the quark mass m_q , we choose $m_q=0.025$ in lattice units in the present analysis. The periodic boundary condition is imposed except for the time direction for the quark fields, which is antiperiodic. We adopt the hybrid R algorithm¹⁰ to update the gauge configuration, in order to treat the $N_f=4$ and 2 cases in parallel, with a molecular-dynamics time step size of $\Delta\tau=0.02$ and one trajectory consisting of 50 time steps. The stopping condition for the quark matrix inversion is $\|\xi - D\chi\|^2/2 \times 3 \times N_s^3 N_t < 10^{-6}$. That this choice of parameters suffices to avoid systematic biases has been checked against a hybrid Monte Carlo run. A time interval of $\tau=8000-10000$ was typically covered at each parameter. The observables were calculated at the end of each trajectory ($\tau=1$). For the chiral order parameter $\langle \bar{\chi}\chi \rangle = \langle \text{tr} D^{-1} \rangle$ we used the noisy estimator. The simulation for the $N_f=2$ system is made by reducing the coefficient of the bilinear noise term by a factor of 2.¹⁰ The errors are estimated by the jackknife method with a bin size of $\delta\tau=950-1000$.

Let us first discuss the result for $N_f=4$. Figure 1 shows the time history of $\text{Re}\Omega$ as a function of τ for

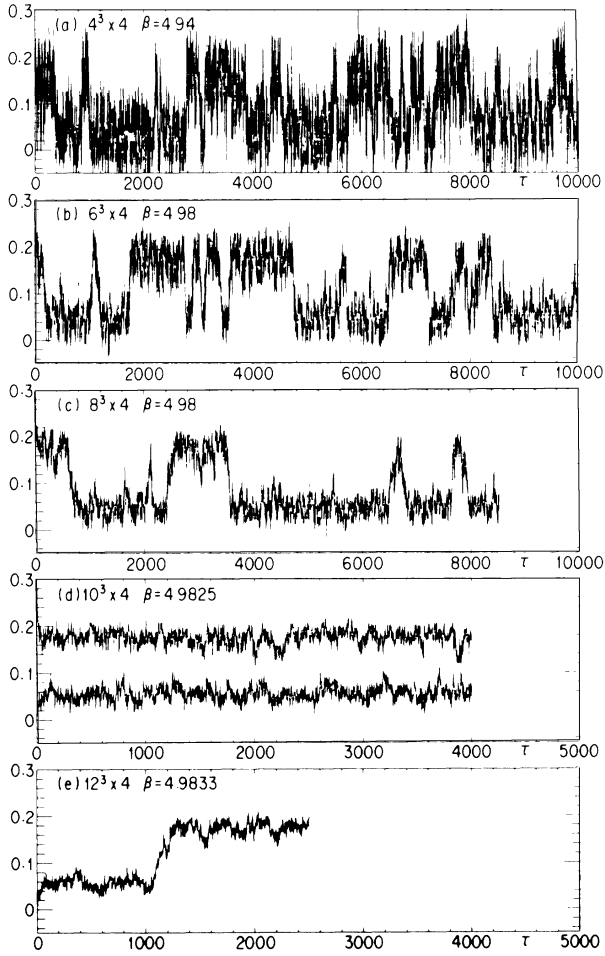


FIG. 1. Time history of the Polyakov line $\text{Re}\Omega$ for $N_f=4$ at $m_0=0.025$ on an $N_s^3 \times 4$ lattice with $N_s=4, 6, 8, 10,$ and 12 .

$N_s=4, 6, 8, 10,$ and 12 . (The time history of $\bar{\chi}\chi$ looks very similar.) We observe distinct flip-flops for $N_s=6$ and 8 , extending the previous observations for $N_s=6$.¹¹ For $N_s=10$ we made two runs from ordered and disordered starts, since we could not observe a flip even for $\tau=4000$. Here we see a clear two-state separation. The behavior is similar for $N_s=12$, where we detected a single flip.¹² For $N_s \geq 6$ the duration of a phase is much longer than the transition time, and fluctuations in each phase are smaller than the gap between the two states. With an increasing volume $V=N_s^3$ the distinction between the two states becomes more pronounced, and the duration of a phase rapidly increases.

We then carry out a finite-size scaling analysis for the susceptibility for the Polyakov line Ω defined by

$$\chi_\Omega = V[\langle (\text{Re}\Omega)^2 \rangle - \langle \text{Re}\Omega \rangle^2]. \quad (3)$$

This analysis requires that the two phases coexist in the sample with a proper weight, which excludes the use of runs for $N_s \geq 10$ not showing flip-flops. The lattice sizes used in the following are hence $N_s=4, 6,$ and 8 . Calcula-

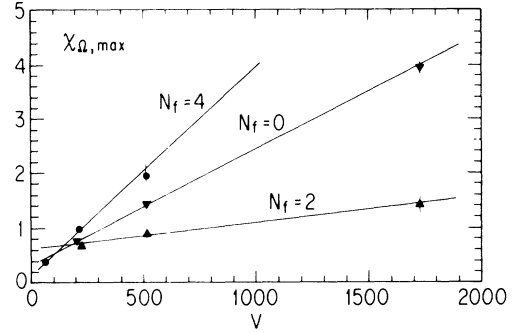


FIG. 2. The peak height of the Polyakov-line susceptibility for $N_f=4, 2,$ and 0 (pure gauge theory) as a function of the spatial volume $V=N_s^3$. The lines are a fit with $\chi_{\Omega,\text{max}}=c+aV$.

ating curves of χ_Ω as a continuous function of β with the spectral-density method,¹³ we estimated the maximum height $\chi_{\Omega,\text{max}}$ of the peak of χ_Ω . The result is shown in Fig. 2, together with a similar plot for $N_f=2$ (to be discussed below) and for the pure SU(3) gauge theory ($N_f=0$) for comparison.

The peak height is expected to scale asymptotically as $\chi_{\Omega,\text{max}} \sim aV^p$. Fitting the data points with this power form gives $p=0.78(4)$. This is less than the first-order value $p=1$.⁷ For the small lattice sizes used here, however, a constant term in the volume dependence of $\chi_{\Omega,\text{max}}$ is not entirely negligible. Indeed, taking $\chi_{\Omega,\text{max}}=c+aV^p$ and making a two-parameter fit for a and p for various values of c (≥ 0), the exponent is found to fall in the range $0.78 < p < 1.1$ for the reduced χ^2 kept within $\chi^2 < 1$ (confidence level > 0.33). We also note that the pure SU(3) gauge theory with a first-order transition⁸ yields $p=0.77(2)$ for a pure power fit and a range of values $0.86 < p < 1.0$ with a constant term for $N_s=6, 8,$ and 12 . Therefore we consider that the size dependence of the peak height obtained here is quite consistent with a first-order nature of the transition.

A similar behavior is also seen in other susceptibilities, χ_P for the average plaquette P and χ_c for the chiral order parameter $\text{tr}(1/D)$. Allowing for a constant term, we obtained $0.68 < p < 1.3$ for $\chi_{P,\text{max}}$ and $0.61 < p < 1.1$ for $\chi_{c,\text{max}}$ with the reduced $\chi^2 < 1$. Fitting all three susceptibilities by the form $c+aV^p$ with a common exponent yields $p=0.90(16)$, with the reduced $\chi^2=0.10$, corresponding to a confidence level of 0.91.

We have also studied the reduced cumulant defined by Challa, Landau, and Binder (CLB),¹⁴

$$V_L = 1 - \frac{1}{3} \frac{\langle P^4 \rangle}{\langle P^2 \rangle^2}. \quad (4)$$

The minimum value of V_L is shown in Fig. 3 as a function of the inverse volume $1/V$. While our lattice size is not sufficiently large, the trend is apparent that $V_{L,\text{min}}$ does not approach $\frac{2}{3}$ as the volume increases, supporting the existence of a discontinuity in the transition.

From this analysis we conclude that the chiral phase

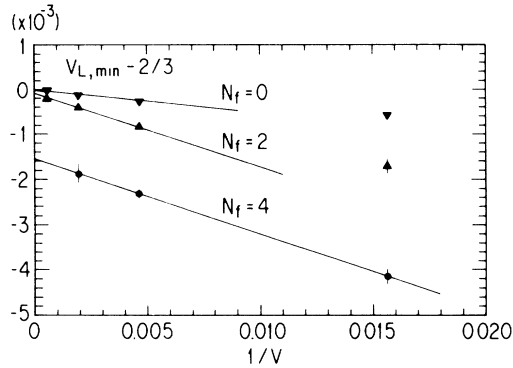


FIG. 3. The minimum value of the CLB cumulant as a function of the inverse volume. The lines are a fit linear in $1/V$ which gives $-1.54(13) \times 10^{-3}$ ($N_f=4$), $-0.95(30) \times 10^{-4}$ ($N_f=2$), and $-1.14(13) \times 10^{-5}$ ($N_f=0$) for $V_{L,\min} - \frac{2}{3}$ at $V = \infty$.

transition for the $N_f=4$ system is consistent with being of first order, and that we have no reason to suspect this conclusion.

Now we turn to the $N_f=2$ case. The time history of $\text{Re}\Omega$ shown in Fig. 4 for $N_s=4, 6, 8,$ and 12 exhibits fluctuations significantly more irregular than the $N_f=4$ case. These fluctuations, if viewed over a short time interval, might have been taken as a two-state signal (e.g., the initial $\tau \sim 2000$ for $N_s=8$). From a long run as we carried out here, however, it is difficult to recognize a clear metastability signal. An increase of the lattice size does not improve the situation.

The size dependence of the peak height of the Polyakov-line susceptibility is presented in Fig. 2 for $N_s=6, 8,$ and 12 . It is possible to fit $\chi_{\Omega,\max}$ with the first-order form $c + aV$ (we find 0.43 for the reduced χ^2). If we allow an arbitrary power of volume ($\chi_{\Omega,\max} = c + aV^p$), however, the data are fitted with a wide range of values $0.32 < p < 1.2$ with the reduced $\chi^2 < 1$ (see Fig. 5 for a plot of the reduced χ^2 vs p). The problem is that the constant term is sizable, and the increase of the peak height from $N_s=6$ to 12 is only by a factor of 2. The trend is similar for $\chi_{P,\max}$ and $\chi_{c,\max}$; the exponents are $0.27 < p < 1.3$ and $0.30 < p < 1.0$, respectively. A simultaneous fit of the three susceptibilities by the form $c + aV^p$ with a common exponent gives $p = 0.55(33)$ (reduced $\chi^2 = 0.025$, or confidence level 0.98).

An analysis of the CLB cumulant (Fig. 3) shows that $V_{L,\min} - \frac{2}{3}$ is substantially smaller than that for $N_f=4$, while it still seems larger than the corresponding value for the pure-gauge case.

From these findings we have to conclude that the chiral phase transition for $N_f=2$ lacks strong evidence for a first-order transition at least at $m_q=0.025$, while our data are not inconsistent with this possibility; the twofold increase of the susceptibility over the lattice sizes accessible to us ($N_s=6-12$) is not large enough to establish it convincingly. It is possible that the present quark

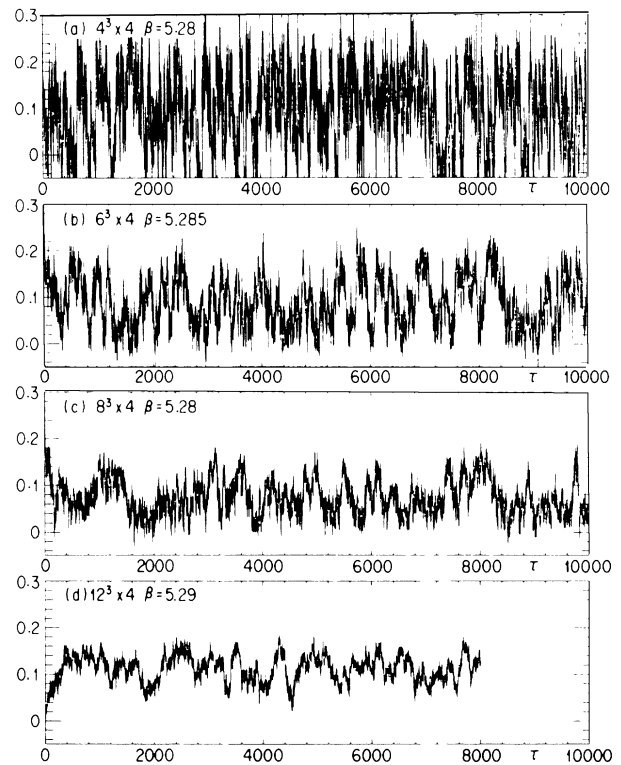


FIG. 4. Time history of the Polyakov line $\text{Re}\Omega$ for $N_f=2$ at $m_q=0.025$ on an $N_s^3 \times 4$ lattice with $N_s=4, 6, 8,$ and 12 .

mass is still too large. For $m_q=0.025$ we suggest, taking the $N_f=4$ case as a guide, that a spatial lattice size of $N_s=24$ or larger will be needed to discriminate the order of the $N_f=2$ transition on a lattice with four time slices.

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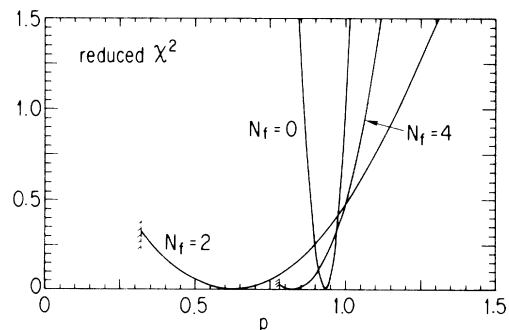


FIG. 5. The reduced χ^2 vs the exponent p for the fit of $\chi_{\Omega,\max}$ by the form $c + aV^p$ with $c (\geq 0)$ a given constant. The constant becomes negative beyond the shade for $N_f=4$ and 2 . The lattice sizes used for the fit are $N_s=4, 6,$ and 8 ($N_f=4$) and $6, 8,$ and 12 ($N_f=2, 0$).

Note added.—After submission of this paper, we extended the analysis of the $N_f=2$ case to a smaller quark mass of $m_q=0.0125$. We found that the system shows characteristics very similar to those for $m_q=0.025$, and we could not determine the order for this case either. The details will be reported elsewhere.

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