Numerical Evidence for a First-Order Chiral Phase Transition in Lattice QCD with Two Light Flavors

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Finite-temperature behavior of quantum chromodynamics with two light dynamical flavors is studied by Langevin simulation on a $8^3\times4$ lattice with the Kogut-Susskind quark action. It is found that the chiral transition strengthens as the quark mass m_q decreases towards zero, changing from a continuous crossover at $m_qa=0.2$ to a first-order transition at $m_qa=0.1$. The critical coupling at $m_q=0$ is estimated to be $\beta_c=6/g_c^2=5.29-5.32$, and the physical scale of $T_c\simeq(0.19-0.24)m_\rho$.

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The dynamics of strong interactions at zero temperature is characterized by quark confinement and spontaneous breakdown of chiral symmetry. It is expected that both these properties will be lost at sufficiently high temperatures, possibly through phase transitions. Quantitative studies of such finite-temperature transitions in QCD have made substantial progress, especially with the recent development of numerical algorithms for incorporating dynamical quarks in the simulation. The results of simulations[1-5] show that the first-order deconfining transition at the pure-gauge-theory limit $m_q=\infty$ weakens with decreasing quark mass m_q, possibly turning into a sharp but continuous crossover for intermediate values of m_q. With further decrease of m_q, however, the transition strengthens again[3] and there is an increasing amount of evidence[3-5] that it becomes a first-order phase transition as m_q approaches the chiral limit $m_q\rightarrow0$.

It should be emphasized that the majority of simulations[3,4] suggesting a first-order chiral transition were carried out for $N_f=4$ degenerate flavors, and the rest[5] were concerned with the case $N_f=3$. It is not known whether this property holds in the physically most relevant case of $N_f=2$ light flavors. In fact a theoretical analysis[6] suggests that the order of the chiral transition might change from first to second as N_f decreases from 3 to 2. It is thus important to carry out an explicit numerical study of the case $N_f=2$, and the purpose of this Letter is to report the result of the first such simulations using the Langevin method on a $8^3\times4$ lattice with the Kogut-Susskind quark action and the single-plaquette gauge action.

Our study shows that the case $N_f=2$ is very similar to the cases with $N_f\geq3$. We found that the transition becomes stronger towards the chiral limit. While the transition appears continuous at $m_qa=0.2$, we found a clear evidence for a two-state signal at $m_qa=0.1$. We therefore conclude that the chiral transition is first order also for $N_f=2$ flavors.

There are several schemes of Langevin simulation.[7,8] For the present work, we used the bilinear noise scheme[8] which allows an arbitrary number of flavors. In this scheme a multiplicative factor of $N_f/4$ in front of the bilinear noise term of the Langevin equation effectively changes the number of flavors to N_f and we set $N_f=2$. We have also used the partial second-order discretization[7] with respect to the fictitious time τ in order to reduce the magnitude of the systematic error due to a finite step size $\Delta\tau$.

Throughout the present work, we used an $8^3\times4$ lattice. This is rather small but should be sufficient for qualitative phase-structure analyses. The bulk of the simulations were carried out with the step size $\Delta\tau=0.01$. Close to the transition region simulations with a smaller step size $\Delta\tau=0.0025$ were also made to ascertain that the nature of the transition does not change with the step size.

We concentrated most of our effort at the quark mass $m_qa=0.1$ and $m_qa=0.2$. To examine the nature of the transition, we first prepare a thermalized configuration at the gauge coupling $\beta=5.7$. The deconfining transition of the pure gauge system occurs at $\beta=5.67\pm0.01$ on an $8^3\times4$ lattice.[9,10] Hence the full QCD system should be in the high-temperature phase at $\beta=5.7$ which indeed was the case for both $m_q a=0.1$ and 0.2. We then cooled the system by decreasing β in steps of $\Delta\beta=0.1$ and mak ing sweeps over $\tau=20$. Measurement of the Polyakov line $\langle\Omega\rangle=\frac{1}{3}\langle\mathrm{tr}\prod U_{n4}\rangle$ and the chiral order parameter $\langle\bar\chi\chi\rangle=\frac{1}{3}\langle\mathrm{tr}D^{-1}\rangle$ with D the lattice Dirac operator for the Kogut-Susskind quarks revealed that the system dropped to the low-temperature phase at $\beta=5.5$–5.4 for $m_q a=0.2$ and $\beta=5.4$–5.3 for $m_q a=0.1$. Once the transition region is thus narrowed down, more detailed studies are made to determine the nature of the transition, with simulations using a longer Langevin time interval and a finer step in β, typically $\tau=50$–200 and $\Delta\beta=0.02$. A less systematic study was made at $m_q a=0.05$, in the region $\beta=5.40$–5.32 with $\tau=50$–100.

In Fig. 1 we show the average value of the Polyakov line and the chiral order parameter at $m_q a=0.2$, 0.1, and 0.05 from the runs with $\Delta\tau=0.01$. Evidently the transition becomes more abrupt with decreasing m_q, and appears discontinuous for $m_q a\leq 0.1$. In order to examine whether the discontinuous behavior at $m_q a\leq 0.1$ signals a first-order transition, we made a thermal-cycle analysis at $m_q a=0.1$ in steps of $\Delta\beta=0.02$ with $\tau=50$. The results, exhibited in Fig. 1 by solid circles, show a clear sign of hysteresis at $\beta=5.38$, suggestive of the first-order nature of the transition at $m_q a=0.1$. To confirm this interpretation we have carried out several additional runs: Starting from the last configuration ($\tau=50$) of the thermal cycle run in the high- (low-) temperature phase at $\beta=5.38$, we cooled (heated) the system to $\beta=5.37$ ($\beta=5.39$). We found that the system quickly moved to the low- (high-) temperature phase. Thus the transition occurs over a narrow range $\beta=5.37$–5.39. We also extended the runs at $\beta=5.38$ from $\tau=50$ to $\tau=250$. The extension from the high-temperature phase showed a single flip-flop to the low-temperature phase (see below for a similar figure with a smaller time step $\Delta\tau=0.0025$). The other run starting from the low-temperature phase, after staying in that phase for a considerable range of τ ($\simeq 200$), moved to the high-temperature phase.

We did not find any signal of metastability at $m_q a=0.2$. The simulations in the region of transition $\beta=5.5$–5.4 at this value of m_q were rather characterized by large and irregular fluctuations as a function of τ and a single broad peak of the histogram. This is illustrated in Fig. 2 which shows the magnitude of fluctuation of the Polyakov line $\sigma^2=\langle(\mathrm{Re}\,\Omega)^2\rangle-\langle\mathrm{Re}\,\Omega\rangle^2$ at $m_q a=0.2$ and 0.1. The existence of a peak for $m_q a=0.2$ strongly contrasts with a relatively flat behavior for $m_q a=0.1$. The same feature also appears in the length of correlation of the Polyakov line and the chiral order parameter in Langevin time τ. If one defines the correlation time τ_r to be the value at which the autocorrelation function decreases to 10% of its value at $\tau=0$, we found that τ_r is small ($\lesssim 1$–2) away from the transition region. We found only a slight increase ($\tau_r\simeq 3$–5) for $m_q a=0.1$

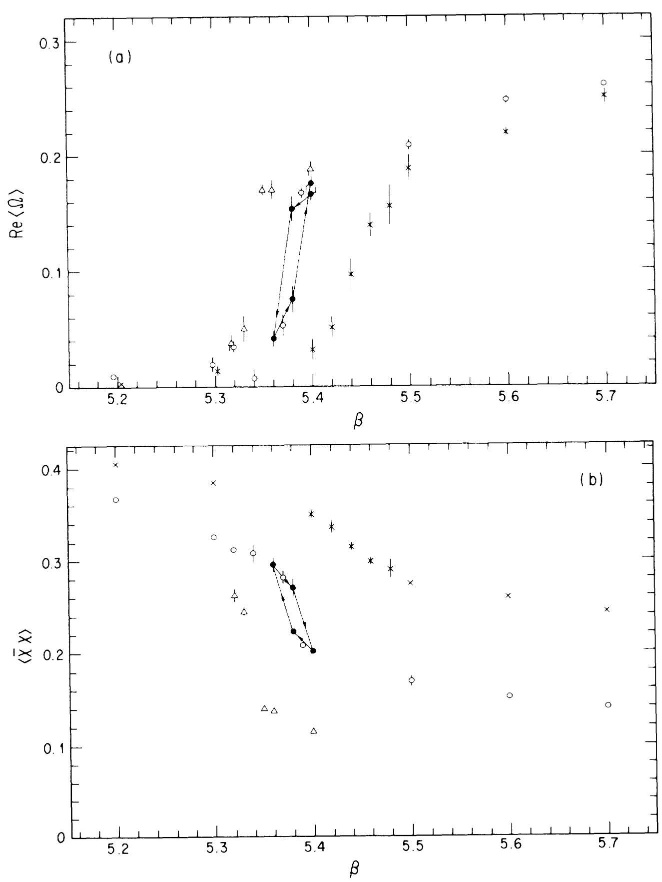

FIG. 1. Average value of (a) the Polyakov line $\mathrm{Re}\langle\Omega\rangle$ and (b) the chiral order parameter $\langle\bar\chi\chi\rangle$ as a function of β for the runs with $\Delta\tau=0.01$. The triangles, circles, and crosses are for the quark mass $m_q a=0.05$, 0.1, and 0.2, respectively. The solid circles show a thermal cycle with $\tau=50$ at $m_q a=0.1$. The errors are estimated taking account of the autocorrelation in τ.

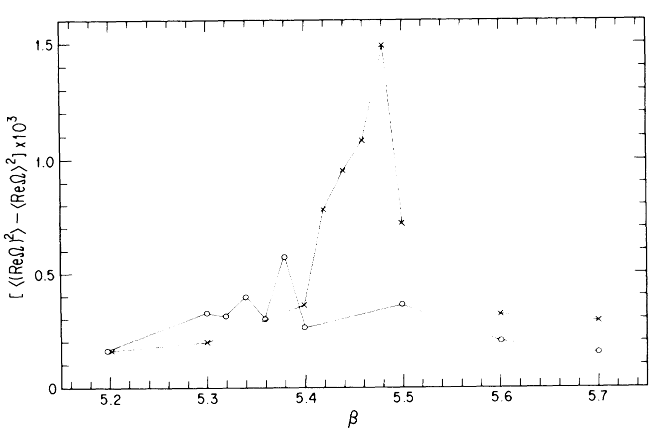

FIG. 2. Variance of the Polyakov line, $\sigma^2=\langle(\mathrm{Re}\,\Omega)^2\rangle-\langle\mathrm{Re}\,\Omega\rangle^2$, for $m_q a=0.2$ (crosses) and $m_q a=0.1$ (circles).

over $\beta=5.3$–5.4 except at $\beta=5.38$ ($\tau_r\simeq20$–25) at which we found signs of metastability. In contrast, at $m_qa=0.2$, τ_r exhibited a broad maximum over $\beta=5.4$–5.5 with $\tau_r\simeq10$. These features are consistent with the transition being first order at $m_qa=0.1$ and continuous or second order at $m_qa=0.2$.

The difference in the behavior of the system between $m_qa\leq0.1$ and $m_qa=0.2$ was also apparent in other observables. In Fig. 3 we show the internal energy density for gluons E_g and quarks E_q calculated by $E_ga^4=3\beta(P_t-P_s)$ with P_t (P_s) the timelike (spacelike) plaquette average and

$$E_qa^4=(N_f/4)(\langle\mathrm{tr}D_tD^{-1}\rangle-\tfrac{3}{4}+\tfrac{1}{4}m_qa\langle\mathrm{tr}D^{-1}\rangle)$$

with D_t the temporal hopping term of D. The continuous change at $m_qa=0.2$ is in marked contrast with the abrupt jump at $m_qa=0.1$ and 0.05.

In the Langevin simulation, a finite step size $\Delta\tau$ introduces a deviation of the action governing the distribution of field configurations. For the Kogut-Susskind quark action, the magnitude of the deviation is of order $\Delta\tau/m_q^2$ and increases with decreasing m_q. It is important to check whether such a deviation might affect the nature of the transition. To examine this point, we carried out simulations at $m_qa=0.1$ decreasing the step size to $\Delta\tau=0.0025$. These runs were generally started from the last configuration of the $\Delta\tau=0.01$ run and were extended over $\tau=50$–200.

Figure 4(a) shows the behavior of the Polyakov line with respect to τ at $\beta=5.3725$. We see nice flip-flops between the low- and high-temperature phases and the histogram in Fig. 4(b) exhibits the corresponding peaks clearly separated. We regard this as strong evidence for the first-order transition at $m_qa=0.1$.

The value of β at which we found evidence of metastability is shifted slightly from $\beta=5.38$ to $\beta=5.3725$ as $\Delta\tau$ is decreased from 0.01 to 0.0025. Also the runs at $\beta=5.375$ and $\beta=5.38$ with $\Delta\tau=0.0025$ were clearly in the high-temperature phase, while the run at $\beta=5.37$ remained in the low-temperature phase (see Fig. 1 for comparison with the $\Delta\tau=0.01$ runs). The direction of the shift agrees with the known result[7,11] that a finite $\Delta\tau$ effectively reduces the value of β. We estimate that the magnitude of the shift with $\Delta\tau=0.01$ is at most $\delta\beta=0.01$, and more importantly, the finite-$\Delta\tau$ effect does not change the nature of the transition.

Let us estimate the critical value β_c at $m_qa=0$. Linear extrapolation of the values $\beta_c=5.37$–5.38 at $m_qa=0.1$ and $\beta_c=5.33$–5.35 at $m_qa=0.05$ gives $\beta_c=5.29$–5.32 at $m_qa=0$. To estimate the physical scale of T_c we utilize the spectroscopy analysis[11] at $\beta=5.5$ (on an $8^3\times18$ lattice) to fix the lattice spacing. Taking into account a correction ($\sim20\%$) due to the difference $\delta\beta\simeq0.2$ by the scaling formula, we obtain

$$T_c/m_\rho=0.19\text{–}0.24 \text{ or } T_c=0.15\text{–}0.18\text{ GeV}.$$

(With this scale $m_qa=0.1$ corresponds to $m_q=60$–80

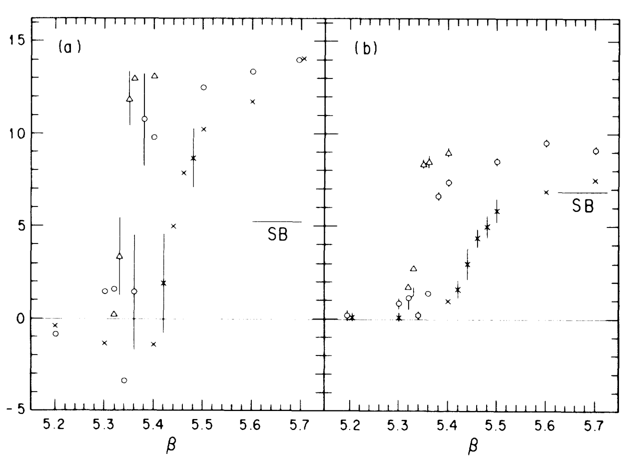

FIG. 3. Internal energy density of (a) gluons and (b) quarks from the runs with $\Delta\tau=0.01$, normalized by the temperature factor T^4 with $Ta=1/N_t=\frac{1}{4}$. The triangles, circles, and crosses represent the data for $m_qa=0.05$, 0.1, and 0.2, respectively. Estimates of autocorrelation time are incorporated in the errors shown. The horizontal bars show the Stefan-Boltzmann value.

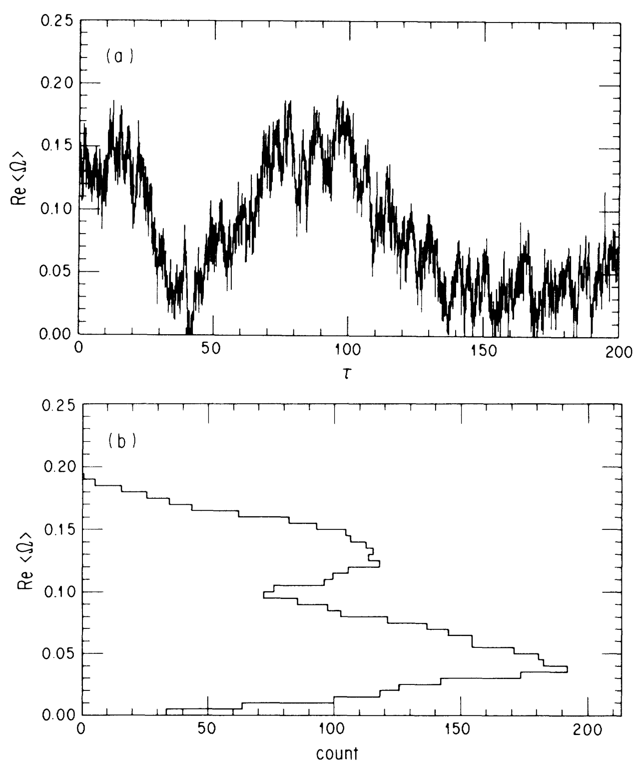

FIG. 4. (a) Langevin time dependence of the Polyakov line $\mathrm{Re}\langle\Omega\rangle$ at $m_qa=0.1$, $\beta=5.3725$ with $\Delta\tau=0.0025$. (b) Histogram for $\mathrm{Re}\langle\Omega\rangle$ for the run exhibited in (a).

MeV.) If we further use the formula

$$\Lambda_L a = (8\pi^2\beta/29)^{345/841}\exp(-4\pi^2\beta/29)$$

for $N_f=2$, β_c may be also translated into $T_c/\Lambda_L = 112-117$ or $T_c/\Lambda_{\overline{\rm MS}} = 2.55-2.66$, in terms of $\Lambda_{\overline{\rm MS}} = 43.88\Lambda_L$.[12] For comparison, we quote $T_c/\Lambda_{\overline{\rm MS}} = 2.55 \pm 0.03$ $(N_f=0)$[9,10] and 2.94 ± 0.22 $(N_f=4)$[3] on a lattice with temporal size $N_t=4$, $T_c/\Lambda_{\overline{\rm MS}} = 2.11 \pm 0.02$ $(N_f=0)$[9] and 2.14 ± 0.10 $(N_f=4)$[13] on a lattice with $N_t=6$.

It is well known that the renormalization-group analysis[6] of an effective meson Lagrangean predicts a first-order chiral transition for $N_f \geq 3$ flavors. The same conclusion actually holds for the case $N_f=2$ if the determinant-type interaction is negligibly small in the region of transition, and in this sense is consistent with our result at $m_q a = 0.1$. The determinant-type interactions are generated by topologically nontrivial gauge configurations (instantons). They are suppressed for light quarks and at high temperatures.[6] Some such suppression might underlie the first-order nature of the chiral transition for $N_f=2$ flavors.

The numerical calculation for the present work was carried out on HITAC S810/10 at the National Laboratory for High Energy Physics (KEK) and on HITAC S810/20 at the Computer Center, University of Tokyo. Three of us (M.F., Y.O., and A.U.) would like to thank the Theory Division of KEK for its warm hospitality. This work is supported in part by the Grants-in-Aid for Scientific Research of the Ministry of Education No. 60790098 and No. 61460019. One of us (S.O.) is supported by the Japan Society for the Promotion of Science.

Note added.—After the paper was submitted we received a preprint by Gottlieb *et al.*[14] who did not find clear signs of metastability with a hybrid algorithm.

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