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Deconfining and Chiral Transitions of Finite-Temperature Quantum Chromodynamics in the Presence of Dynamical Quark Loops

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Finite-temperature behavior of quantum chromodynamics is investigated with the Langevin technique including the dynamical quark loops. The deconfining and chiral transitions occur at the same temperature. The strength of transition weakens initially as the quark mass decreases from infinity, but at small quark masses it strengthens again and shows the characteristic of a first-order transition. We estimate the inverse coupling constant at zero quark mass to be $\beta_c = 6/g_c^2 \simeq 4.9-5.0$ for four flavors on an $8^3 \times 4$ lattice.

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It is an important question of quantum chromodynamics to ask how the two basic features of hadron dynamics at zero temperature, confinement of quarks and spontaneous breakdown of chiral symmetry, will disappear as temperature increases. For the pure SU(3) gauge system the finite-temperature behavior is now well established: It has a first-order phase transition separating the low-temperature confining phase from the high-temperature plasma phase.[1] It has also been shown within the quenched approximation that the restoration of chiral symmetry takes place precisely at the deconfining temperature.[2] The coupling of quarks introduces several nontrivial problems. For heavy quarks it has been shown that the effect of quark loops weakens the deconfining transition and that its location shifts towards weaker couplings.[3] One of the questions is whether there remains a first-order phase transition for light quarks. On the other hand, we expect for a zero-mass quark the spontaneous breaking of chiral symmetry. It has been shown in the σ-model analysis that there exists a first-order chiral transition for the number of flavors $N_F \geqslant 3$.[4] We expect that this transition would also become weak or might even disappear when the mass of quarks becomes large. The relation between these two transitions is also to be understood.

There already exist several numerical analyses attempting to clarify these issues.[5] However, the nature of the transition for light quarks is still controversial. In addition to the poor overall statistics, the approximations used in the formalism for including dynamical quark loops make it difficult to draw a definite conclusion from the simulations made so far.

In this Letter we attempt to elucidate the nature and interplay of the deconfining and chiral phase transitions as a function of quark masses in the presence of dynamical quark loops. We have applied the Langevin technique[6,7] to the SU(3) gauge system with the Kogut-Susskind action having $N_F = 4$ flavors on an $8^3 \times 4$ lattice. The advantage of this method is that it does not involve approximations which could cause unknown systematic biases and that the error of the simulation is in principle under control. We have examined the behavior of the system for a variety of quark masses by carrying out the thermal cycle analysis in the coupling constant at fixed quark masses. The calculation took 350 h on the HITAC S-810/10 at KEK [average operational speed is about 150 Mflops

(flops = floating-point operations per second)] and 70 h on the S-810/20 at the University of Tokyo (~300 Mflops).

Our simulation shows that the deconfining transition at $m_q = \infty$ smoothly continues into the region of small m_q. The strength of the transition initially weakens when the quark masses decrease from $m_q = \infty$, and for $m_q \simeq 0.2$–0.3 we cannot conclude the presence of a first-order phase transition. For smaller m_q, however, the transition becomes stronger again and exhibits the nature of a first-order phase transition at $m_q = 0.1$. Across this transition both the chiral order parameter $\langle\bar{\chi}\chi\rangle$ and the Polyakov line $\langle\Omega\rangle$ simultaneously jump, with the jump of the former becoming progressively pronounced for smaller m_q.

We now describe the simulation in some detail. The effective action is given by

$$S_{\rm eff} = -\frac{\beta}{6}\sum_p {\rm tr}(U_p + U_p^\dagger) + Y^\dagger \frac{1}{D^\dagger D} Y, \qquad (1)$$

where the first term represents the standard single plaquette action for the gauge variable $U_{n\mu}$, and Y_n denotes the pseudofermion variable with

$$D_{n,n'} = m_q \delta_{n,n'} + \tfrac{1}{2}\sum_\mu \eta_{n\mu}(U_{n\mu}\delta_{n,n'+\hat{\mu}} - U^\dagger_{n'\mu}\delta_{n,n'-\hat{\mu}}) \qquad (2)$$

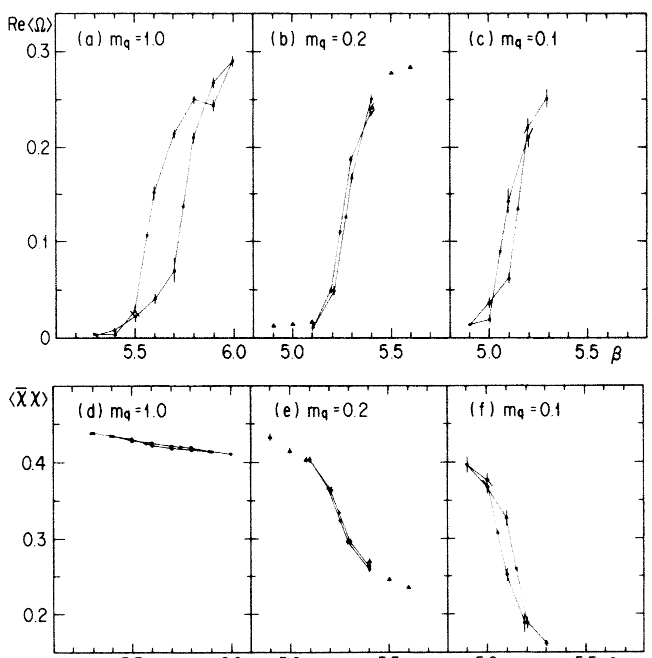

FIG. 1. Average values of (a)–(c) temporal Polyakov line $\mathrm{Re}\langle\Omega\rangle$ and (d)–(f) the chiral order parameter $\langle\bar{\chi}\chi\rangle$ as functions of β at $m_q = 1.0$, 0.2, and 0.1 in thermal-cycle runs. Average is taken for $10 \leq \tau \leq 20$ ($\Delta\tau = 0.002$ for $m_q = 0.1$ and 0.2, and $\Delta\tau = 0.01$ for $m_q = 1.0$). Errors shown are statistical, estimated by taking account of the data of autocorrelations. Triangles in (b) and (e) show the averages for different runs with $\Delta\tau = 0.01$.

representing the Kogut-Susskind quark action. In order to reduce the number of flavors to four, we used the trick of setting $Y_n = 0$ on odd sites.[8] We refer to Ref. 6 for the form of the Langevin equation and its discretization in the fictitious time.

We have carried out the thermal cycle in β in steps of $\Delta\beta = 0.1$ at $m_q = 0.1$, 0.2, 0.3, 0.5, and 1.0, and $20/\Delta\tau$ iterations are made at each β with the Langevin time step $\Delta\tau = 0.01$–0.002, depending on m_q.[9] We have checked that this is enough for thermalization. The observables depending only on gauge variables were calculated at every $\delta\tau = 0.1$ and those depending on quarks at every $\delta\tau = 0.2$. For the latter we computed $(D^{-1})_{n,n_0}$ for sixteen n_0's with the coordinate either at the origin or at the midpoint along the axis. The last $10/\Delta\tau$ iterations were used for the average.

In Fig. 1 we show the average of the temporal Polyakov line defined by $\Omega = {\rm tr}(\prod U_{n4})/3$ and the chiral order parameter $\langle\bar{\chi}\chi\rangle = \langle{\rm tr}D^{-1}\rangle/3$ at several values of the quark mass m_q. It is seen that these quantities jump or change rapidly when we heat up (or cool down) the system. Figure 2 summarizes the position of β at which the jump happened as a function of m_q.

For a large enough m_q, e.g., $m_q = 1.0$ ($m_q/T_c = 4.0$) the observed hysteresis ($\beta = 5.5$–5.8) is consistent with the first-order phase transition for pure gauge system which occurs at $\beta = 5.66$–5.68.[10] As m_q decreases, the hysteresis of the thermal cycle weakens, and it disappears at $m_q \simeq 0.3$ ($m_q/T_c \simeq 1.2$). This reflects the weakening of the first-order deconfining transition due to the $Z(3)$-breaking perturbation of dynamical heavy quarks.[3]

When we further decrease the quark mass to $m_q = 0.1$ ($m_q/T_c = 0.4$), however, we again observe the hysteresis. To see this point more carefully, we extended our runs to 2×10^4 iterations ($\tau = 40$), and in

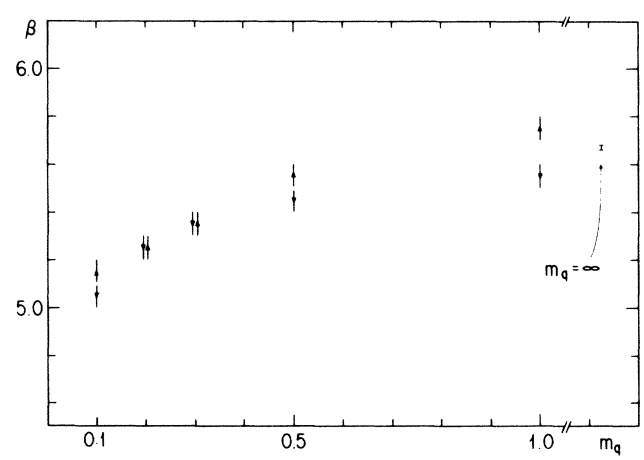

FIG. 2. Phase diagram of the deconfining and chiral phase transitions in (m_q, β) plane. The upward (downward) arrow shows the position of β at which $\mathrm{Re}\langle\Omega\rangle$ and/or $\langle\bar{\chi}\chi\rangle$ jump, or change rapidly, in the heating (cooling) cycle.

Fig. 3 we present $\mathrm{Re}\langle\Omega\rangle$ at every 500 iterations for $m_q=0.1$ and $\beta=5.1$ in our heating and cooling cycles. One can see that in the two runs the $\mathrm{Re}\langle\Omega\rangle$ do not show the trend of approaching each other. Probably the most subtle point concerning the hysteresis analysis is the question of critical slowing down towards light quark masses. We examined the autocorrelation of the Polyakov line, Wilson loops, and $\bar{\chi}\chi$ while carrying out the thermal-cycle analysis, and found that the relaxation time τ_r of the Polyakov line, defined to be that at which the autocorrelation decreases to 10% of its value at $\tau=0$, is $\tau_r\sim 1$ for $m_q\gtrsim 0.2$ and $\tau_r=3$–4 for $m_q=0.1$ in the respective critical regions (similar numbers are also obtained from the other physical quantities). We found from the data for $m_q=0.2$–1.0 that, if there are no metastable states, the heating and cooling data approach each other already at $\tau\sim(5$–$6)\tau_r$. Our data at $m_q=0.1$ do not show any such tendency even after $\tau/\tau_r=40/\tau_r\sim 10$. Therefore we regarded this as evidence that the phase transition is first order.

The strengthening of the hysteresis in the Polyakov loop towards smaller quark masses is accompanied by an increasingly discontinuous behavior of the chiral order parameter $\langle\bar{\chi}\chi\rangle$. In Fig. 4 we plot the value of $\langle\bar{\chi}\chi\rangle$ at couplings just above and below the hysteresis region. The value of $\langle\bar{\chi}\chi\rangle$ is smaller on the weak-coupling (high-temperature) side of the transition with its magnitude diminishing rapidly with the quark mass, while it stays finite on the strong-coupling (low-temperature) side. The gap across the transition decreases approximately as $\sim m_q^{-1}$, as expected. The restoration of chiral symmetry is thus the main characteristic of the transition at small quark masses, and these observations lead us to conclude that the chiral transition at $m_q=0$ is of first order and that it remains so for a range of finite m_q.

We should also note that the jump of $\langle\Omega\rangle$ occurs exactly at the point where $\langle\bar{\chi}\chi\rangle$ changes discontinuously: The deconfining and chiral phase transitions always occur simultaneously for the quark in the fundamental representation.

Let us now compare our result at the lightest quark mass $m_q=0.1$ with those in the literature for $N_F=4$.[5] Our data of $\langle\Omega\rangle$ and $\langle\bar{\chi}\chi\rangle$ agree very well with those of Polonyi *et al.*[11] (even at $\beta=5.1$, where a rapid change of physical quantities was observed in Ref. 11). They also agree well with those of Gavai,[12] except for the transition region, which is shifted upwards by $\Delta\beta\simeq 0.06$ in Ref. 12. These authors did not make claims on the existence or absence of the first-order phase transition (some indication for weak metastability was reported in Ref. 12). A merit of the present analysis may be the fact that we have carried out a controlled thermal-cycle analysis, which is likely to be better than simply comparing runs with a cold and a hot start for detecting the metastable state.

To fix the mass scale in physical units, it is necessary to carry out a hadron-mass calculation in the presence of dynamical quarks. A rough estimate, however, can be made by assuming the scaling as follows: With the aid of

$$a\Lambda_L=(8\pi^2\beta/25)^{231/625}\exp(-4\pi^2\beta/25) \quad (3)$$

for $N_F=4$, the deconfining transition temperature $aT_c=\frac{1}{4}$ can be expressed in terms of Λ_L, or of $\Lambda_{\overline{\mathrm{MS}}}$ ($\overline{\mathrm{MS}}$ denotes the modified minimal-subtraction scheme) with the use of[13] $\Lambda_{\overline{\mathrm{MS}}}/\Lambda_L=76.44$ ($N_F=4$). The transition temperature at $m_q=0.1$ is then $T_c/\Lambda_{\overline{\mathrm{MS}}}\simeq 3.68$ and $m_q/\Lambda_{\overline{\mathrm{MS}}}\simeq 1.47$.

Let us estimate T_c for $m_q=0$. Making an extrapola-

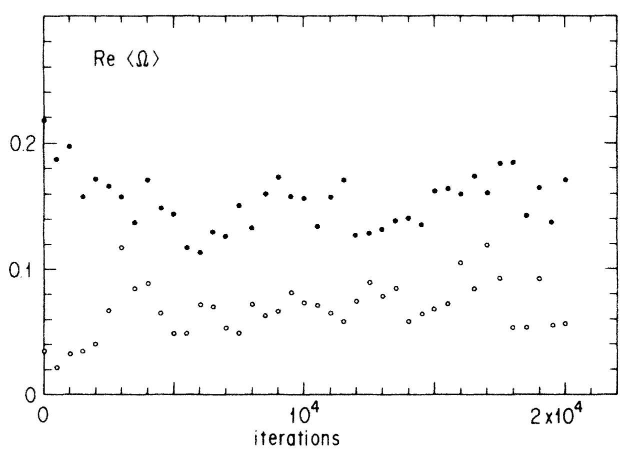

FIG. 3. $\mathrm{Re}\langle\Omega\rangle$ at every 500 iterations with the time step $\Delta\tau=0.002$ at $m_q=0.1$ and $\beta=5.1$. Solid (open) circles denote data in the cooling (heating) thermal cycle.

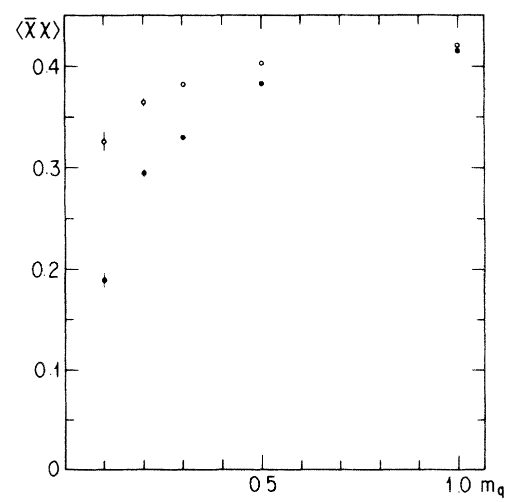

FIG. 4. The value of $\langle\bar{\chi}\chi\rangle$ along the transition line. Solid (open) circles show the value of β just above (below) the jump of $\langle\bar{\chi}\chi\rangle$ in the heating cycle.

tion in Fig. 2 gives $\beta_c \approx 4.9$–5.0 at $m_q = 0$, and we find $T_c/\Lambda_{\overline{\rm MS}} \approx 2.7$–$3.1$. This value may be compared with that obtained for a pure gauge system on an $8^3 \times 4$ lattice: $T_c/\Lambda_{\overline{\rm MS}} = 2.6$.[10] The agreement between these two values seems to be fortuitous, because a large modification in $a\Lambda_L$ naively expected from the change $\Delta\beta \approx 0.8$ happens to be canceled by a change of the beta-function coefficients and also by a modification in $\Lambda_{\overline{\rm MS}}/\Lambda_L$.

Of course, the values of T_c/Λ quoted above should be taken as only indicative, because our lattice size is probably not large enough to extract physics in the continuum and a sizable violation of scaling may be expected. In order to address these quantitative questions, rather than the elucidation of the nature of the transition aimed at in the present work, simulations on a larger lattice are clearly needed.

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