Finite-Temperature Phase Structure of Lattice QCD with the Wilson Quark Action for Two and Four Flavors

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We present further analyses of the finite-temperature phase structure of lattice QCD with the Wilson quark action based on spontaneous breakdown of parity-flavor symmetry. Results are reported on (i) an explicit demonstration of spontaneous breakdown of parity-flavor symmetry beyond the critical line, (ii) phase structure and order of chiral transition for the case of \( N_f = 4 \) flavors, and (iii) approach toward the continuum limit.

1. Introduction

Elucidating the finite-temperature phase structure of lattice QCD with the Wilson quark action is complicated by the fact that the action explicitly breaks chiral symmetry [1]. Last year we reported an analysis of this problem [2] based on the idea of spontaneous breakdown of parity and flavor symmetry [3]. The main findings, obtained through simulations of the two-flavor system on an \( 8^3 \times 4 \) lattice, were that (i) the critical line, defined as the line of vanishing pion screening mass for finite temporal lattice sizes, does not extend to arbitrarily weak coupling, but turns back toward strong coupling at a finite value of \( \beta \), forming a cusp on the \((\beta, K)\) plane, and (ii) the thermal line of finite-temperature transition \( K = K_t(\beta) \) runs past the tip of the cusp without crossing the critical line.

We have also argued, based on analytical considerations including those of the two-dimensional Gross-Neveu model, that the cusp will move to weak coupling as the temporal size \( N_t \) increases, pushing the thermal line in front and eventually pinching it at \( K = 1/8 \) and \( \beta = \infty \) as \( N_t \to \infty \). In our view it is only in this limit that the true chiral phase transition emerges.

While this view provides a consistent picture on how chiral phase transition arises for the Wilson quark action, we have left unanswered several important questions to be clarified. These are (i) an explicit demonstration that parity-flavor symmetry is spontaneously broken inside the cusp, (ii) how the phase diagram depends on the number of flavors \( N_f \), in particular if the chiral transition is of first order for \( N_f \geq 3 \) as predicted by the sigma model analysis, and (iii) how the tip of the cusp moves for an increasing temporal lattice size. In this article, we present results of our study on these questions carried out since last year.

2. Evidence for spontaneous breakdown of parity-flavor symmetry

Spontaneous breakdown of parity-flavor symmetry inside the cusp is signaled by a non-vanishing vacuum expectation value of the pion field. For the case of two flavors \( N_f = 2 \) which we analyze, one may take the pion condensate to point in the \( \tau_3 \) direction \(< \bar{\psi} i \gamma_5 \tau_3 \psi > \neq 0 \). The pion spectrum will then consist of a massive \( \pi^0 \) and massless \( \pi^\pm \) which are the Nambu-Goldstone modes of the broken symmetry.

In order to ascertain these predictions we carry out hybrid Monte Carlo (HMC) simulations, adding a symmetry-breaking term \( \delta S_W = 2K H \sum_n \bar{\psi}_n i \gamma_5 \tau_3 \psi_n \) to the action to avoid infrared divergences due to massless \( \pi^\pm \) modes.

Runs are made on an \( 8^3 \times 4 \) lattice at \( \beta = 3.5 \) with \( 0.21 \leq K \leq 0.28 \) in steps of 0.01. The range for the hopping parameter includes the interval \( K_c = 0.2267(2) \leq K \leq 0.2463(7) = K_c' \) previously estimated to be the parity broken phase [2]. For the external field we take \( H = 0.2, 0.1, 0.05, 0.02 \) and 0.01. For each value of \( K \) and \( H \), typically 20 – 50 trajectories with 0.5 time units are made for thermalization followed by 50 trajectories for measurements. The presence of ex-
ternal field significantly reduces fluctuations, and we find these statistics to be sufficient. Hadron screening masses are calculated by periodically doubling the lattice in the spatial directions.

In fig. 1 we plot the parity-flavor order parameter \( <\bar{\psi}\gamma_5\gamma_3\psi> \) as a function of \( 1/K \) for \( \beta = 3.5 \) on an \( 8^3 \times 4 \) lattice for \( N_f = 2 \).

Similarly, the \( \pi^\pm \) screening mass squared is plotted in fig. 2(a) as a function of \( 1/K \) and in fig. 2(b) as a function of \( H \). Inside the cusp \( m_{\pi^\pm}^2 \) decreases toward zero, while outside it converges toward values calculated with \( H = 0 \) (open squares). For \( K_c = 0.23 \) and 0.24, which are inside the cusp, lines in fig. 2(b) show quadratic fits of form \( m_{\pi^\pm}^2 = A + BH + CH^2 \). A small non-vanishing value of the intercept \( A \approx 0.02 \) is ascribed to finite spatial size effects.

We conclude that the behavior of both the parity-flavor order parameter and \( m_{\pi^\pm}^2 \) strongly supports spontaneous breakdown of parity-flavor symmetry inside the cusp.

An interesting point to note is that \( m_{\pi^\pm}^2 \) converges to the limit \( H = 0 \) from below for \( K > K_c \), while the approach is from above for \( K < K_c \). In other words, the parity-flavor broken phase is enlarged beyond the upper part of the critical line in the presence of the external field.

We also mention that extracting the \( \pi^0 \) mass inside the cusp requires computation of disconnected quark loop contribution in the \( \pi^0 \) propagator. This may be carried out with the technique of wall source without gauge fixing previously applied to the \( \eta' \) propagator \cite{4}. We leave this interesting problem for future work.

3. Phase diagram for the case of \( N_f = 4 \)

Our analysis of the \( N_f = 4 \) system is made for the dual purpose of confirming the cusp structure of the critical line and examining the dependence of the order of chiral transition on \( N_f \).

HMC runs with \( H = 0 \) are carried out on an \( 8^3 \times 4 \) lattice at \( 0 \leq \beta \leq 4.0 \) and \( 0.19 \leq K \leq 0.30 \). Thermalization of 20 – 50 trajectories with 0.5 time units followed by 50 – 100 trajectories for measurements are made at each \( \beta \) and \( K \), chaining runs in \( K \) for each value of \( \beta \). The location of the critical line is estimated from results of \( m_\pi^2 \) calculated on a spatially doubled lattice, and the
Figure 3. Phase diagram for the $N_f = 4$ system for $N_t = 4$. Previous result for $N_f = 2$ is also shown for comparison. Solid lines are critical lines and dotted lines the line of thermal transition. Solid squares mark points where first-order signals are found, while open rectangles represent region of smooth crossover.

Position and order of the thermal transition is examined through behavior of physical quantities and their time histories.

In fig. 3 we show the phase diagram for $N_f = 4$ together with that for $N_f = 2$ previously reported\cite{2}. We find a cusp structure similar to that of $N_f = 2$ except for a shift of $\delta \beta \approx 1.2$ toward stronger coupling, which we qualitatively expect from a larger magnitude of sea quark effects for $N_f = 4$. We also find strong first-order signals across the thermal line away from the tip of the cusp as marked by solid squares. Surprisingly, however, the transition becomes weaker toward the tip of the cusp, apparently turning into a smooth crossover at $\beta = 2.5 - 2.0$. The location of the crossover is indicated by open rectangles in fig. 3.

The smoothing of the transition close to the cusp is illustrated in fig. 3(a) for $m_\pi^2$ and in (b) for the Polyakov line $\Omega$. Jumps in physical quantities are apparent at $\beta = 4.0$ and 3.5. However, at $\beta = 2.5$ and 2.0, data taken for increasing and decreasing values of $K$ overlap with each other and do not show any sign of discontinuity.

At $\beta = 2.0$ runs are also made with an increased spatial size of $12^3 \times 4$. Results for $m_\pi^2$ plotted by open circles do not show deviation from those on an $8^3 \times 4$ lattice. Thus it is unlikely that finite-size effects has rounded a first-order discontinuity into a smooth crossover on an $8^3 \times 4$ lattice.

A possible interpretation of the smoothing is that it is caused by an explicit breaking of chiral symmetry in the Wilson quark action, whose effect is larger for stronger coupling. If one increases the temporal lattice size $N_t$, the cusp and the line of thermal transition will both move toward weaker coupling. Therefore the first-order transition may become extended up to and beyond the tip of the cusp for sufficiently large $N_t$.

Another possibility is that the first-order transition we find is a lattice artifact, sharing its origin with the sharpening of the $N_f = 2$ transition observed at $\beta \approx 5.0$\cite{5}. This possibility does not contradict the report of a first-order transition for $N_f = 3$\cite{6}. In fact the interval $4.0 \leq \beta \leq 4.7$ where first-order signals were observed is away from the cusp expected at $\beta \approx 3.0$. Also we think that the divergence of runs at $\beta \approx 3.0$ from a hot
and a mixed starting configurations reported in ref. [6] is an indication that the runs were made inside the parity-broken phase rather than a signal of metastability.

For either of the two possibilities above, if the chiral phase transition is of first order for \( N_f \geq 3 \) in the continuum, it will emerge only for larger \( N_t \) for which the cusp and the thermal line move into the scaling region toward weak coupling.

4. Approach toward the continuum limit

Discussions of the previous section naturally raise the question how the cusp of the critical line moves when the temporal lattice size is increased. To examine this problem, we analyze the critical line for an \( 8^3 \times 8 \) lattice for \( N_f = 2 \) and 4 systems. We do not repeat a description of simulation details since they are similar to those for an \( 8^3 \times 4 \) lattice.

In fig. 5 we plot the critical line estimated from the pion mass. We observe that the cusp is clearly shifted toward weak coupling. However, the magnitude of shift is quite small both for \( N_f = 2 \) and 4 so that the tip of cusp is still in the region of strong coupling for \( N_t = 8 \). Let us note that previous results by the QCDPAX Collaboration for \( N_f = 2 \) also indicate that the tip of the cusp is located at \( \beta = 4.0 - 4.2 \) for \( N_t = 6 \) and at \( \beta = 4.5 - 5.0 \) even for \( N_t = 18 \). A recent study on a symmetric lattice employing parity-flavor breaking external fields also shows that the cusp is located below \( \beta = 5.0 \) up to \( N_t = 10 \). These results imply that a substantial increase in the temporal lattice size is needed before the cusp and the thermal line move into the scaling region (e.g., \( \beta \geq 5.5 \) for \( N_f = 2 \)).

We should emphasize that this result has a significant impact also for spectrum calculations at zero temperature. Since the location of the cusp is controlled by the smaller of the temporal and spatial lattice sizes, unless the spatial size is taken sufficiently large, critical hopping parameter will be absent, leading to systematic errors in measured hadron masses.

Overall our study indicates that within the plaquette gauge action and the Wilson quark action large lattice sizes are needed for an exploration of continuum properties of the chiral phase transition. The associated computational difficulties point toward application of improvement ideas [8,9] to achieve further progress in finite-temperature studies with the Wilson-type quark actions.

We thank Y. Iwasaki, K. Kanaya and T. Yoshié for useful discussions. This work is supported in part by the Grants-in-Aid of the Ministry of Education (Nos. 04NP0801, 08640349, 08640350).

REFERENCES

1. M. Fukugita, S. Ohta and A. Ukawa, Phys. Rev. Lett. 57 (1986) 1974; A. Ukawa, Nucl. Phys. B(Proc. Suppl.)9 (1990) 463.
2. S. Aoki, A. Ukawa and T. Umemura, Phys. Rev. Lett. 76 (1996) 873; Nucl. Phys. B(Proc. Suppl.)47 (1996) 511.
3. S. Aoki, Phys. Rev. D30 (1984) 2653; Phys. Rev. Lett. 57 (1986) 3136; Nucl. Phys. B314 (1989) 79.
4. N. Kuramashi et al., Phys. Rev. Lett. 72 (1994) 3448.
5. C. Bernard et al., Phys. Rev. D46 (1992) 4741, 49 (1994) 3574, 50 (1994) 3377.
6. Y. Iwasaki et al., [hep-lat/9605030].
7. K. M. Bitar, [hep-lat/9602027].
8. Y. Iwasaki et al., Nucl. Phys. B(Proc. Suppl.) 42 (1995) 502; ibid 47 (1996) 515.
9. MILC Collaboration (presented by M. Wingate ), this volume.