Is the 2-Flavor Chiral Transition of First Order?

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We study the effects of the interaction between the Chiral condensate and the Polyaev loop
on the chiral transition within an effective Lagrangian. We find that the effects of the interaction
change the order of the phase transition when the explicit breaking of the $Z_N$ symmetry of the
Polyakov loop is large. Our results suggest that the chiral transition in 2-flavor QCD may be first
order.

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I. INTRODUCTION

QCD matter with $N_f$ flavors, $N$ colors and zero baryon chemical potential undergoes
two finite temperature phase transitions, the chiral transition and the deconfinement. The chiral transition is
associated with the spontaneous breaking of the chiral symmetry, $SU(N_f)_L \times SU(N_f)_R$, below the critical
temperature ($T_c$) for massless quarks. The order parameter for this transition is the chiral condensate. On
the other hand the deconfinement transition is associated with the spontaneous symmetry breaking,$Z_N \times SU(N)$ at above the critical temperature $T_d$ for infinitely heavy quarks. The order parameter for the transition is the Polyakov loop expectation value. For
finite non-zero quark masses both the chiral symmetry and the $Z_N$ symmetry are explicitly broken. Nevertheless these two transitions show up as crossover, second order transitions depending on
the values of the quark masses. The chiral transition depends on the number of quark flavors
and the deconfinement transition depends on the number of colors. Since the chiral symmetry and
the $Z_N$ symmetry seem nothing to do with each other one would expect that these two transitions occur independently. However lattice QCD calculations have shown that both these transitions occur simultaneously, $T = T_d$ [1-5]. Furthermore strong correlation between the chiral condensate and
the Polyakov loop is observed around the phase transition point [6]. This is clear evidence that there is
interaction between these two order parameters. So studying the interaction between the chiral
condensate and the Polyakov loop is fundamental for understanding the interplay between the chiral
transition and deconfinement. There are several studies on the possible causes of the simultaneous
occurrence of the chiral transition and the deconfinement transition. Mixing the gauge and matter
operators has been suggested to explain the simultaneous chiral and deconfinement transitions [7,8]. Some other studies consider that for small quark masses the chiral transition drives
the deconfinement transition [9,10].

Though most of the studies are concerned with why $T = T_d$ only a few have considered the effect of the interaction on the phase transition itself [11]. It seems natural to expect that if the interaction between the two order parameters result in the simultaneous occurrence of the two transitions then the interaction may also have important effect on the phase transition. One of the most
interesting cases to study for the possible effects of this interaction is the 2-flavor chiral transition.
Lattice QCD calculations have not yet been able to settle on the order of this phase transition.
Lattice calculations by different groups do not agree on the order of this phase transition. Some lattice groups find the transition is second order [3] and other groups find the transition is first order [11]. Conventionally this transition is believed to be second order and in the universality class of the O(4) Heisenberg magnet [12]. But the effect of interaction between the chiral order parameter \( \chi \) and the Polyakov loop \( L \) may change the behavior of this transition. So in the present work, we investigate the effect of interaction between \( \chi \) and \( L \) on the 2-flavor chiral transition within an effective Lagrangian.

Previously, the effect of interaction between the chiral order parameter and the Polyakov loop has been studied in the renormalization group approach [5]. The main difference between the present work and previous studies is that we consider the explicit breaking of the \( Z_N \) symmetry. Explicit breaking of the \( Z_N \) symmetry can be introduced in the effective Lagrangian by terms such as \( (L + L')^y \). Previous studies [10] have considered interaction terms such as \( (LL')^y \), which respects the chiral and the \( Z_N \) symmetry. However, in the chiral limit, the interaction terms need not respect the \( Z_N \) symmetry. So terms such as \( (L + L')^y \) should be considered. As we discuss later, such an interaction term is always present if the explicit \( Z_N \) symmetry breaking is large, for example in the chiral limit. For simplicity, we consider \( N = 2 \) color QCD. We expect that different \( N \) will not qualitatively change the physics we are discussing here. For \( N_f = 2 \), the chiral order parameter is a four component vector field whereas for \( N = 2 \), the Polyakov loop \( L \) is a real scalar field. In this work, we basically study the effect of the three terms \( s, L, L' \) and \( L^2 \) in the effective Lagrangian. Our main result is that the strong explicit breaking of the \( Z_N \) symmetry can make the chiral transition first order. We show that the chiral transition can be first order even at the mean field level. We also carry out numerical Monte Carlo simulations which confirm the first order phase transition for large enough explicit \( Z_N \) symmetry breaking. We mention here that the \( N_f = 2 \) chiral transition can be first order from the interaction term \( L^2 \) without \( Z_N \) symmetry breaking [11]. However, lattice QCD results indicate that the effect of the \( Z_N \) symmetry breaking is small. A possible first order chiral transition can result more likely from the explicit \( Z_N \) symmetry breaking as we will argue later.

Conventionally explicit symmetry breaking weakens a phase transition. But our results suggest that for a system with two order parameter fields, explicit symmetry breaking can make the transition stronger. It is interesting to note that the chiral order parameter does not couple to gauge fields directly. The gauge fields seem to act the chiral phase transition indirectly through the Polyakov loop. We mention here that the effect of explicit symmetry breaking discussed here should not be restricted to the \( Z_N \) symmetry. We expect that the explicit breaking of chiral symmetry may have some effect on the deconfinement transition in the large quark mass region. We mention here that interaction between the chiral order parameter and the diquark field is considered to study the chiral/color-superconducting transition at low temperature and high density [13].

This paper is organized as follows. In section-II we describe the effective Lagrangian and discuss the effect of the interaction between \( \chi \) and \( L \) on the chiral transition. We describe our numerical Monte Carlo calculations and results in section-III. The discussions and conclusions are presented in section-IV.

II. THE EFFECTIVE LAGRANGIAN AND THE EFFECT OF THE BROKEN \( Z_N \) SYMMETRY

We consider the following Lagrangian [3] in 3 dimensions for the \( \chi \) and \( L \) fields,
The parameters to find correspond to a degenerate minimum of the effective potential \( V(\mu; L) \), which breaks the \( Z_2 \) symmetry explicitly. The interactions between the chiral order parameter and the Polyakov loop are taken care of by the fifth and sixth terms in \( V(\mu; L) \).

The signs of the couplings \( g \) and \( e \) decide the correlation between the fluctuations of the \( \mu \) and \( L \) fields. For example, when \( c > 0 \), the themal average of the correlation between the \( \mu \) fluctuations, \( h(\mu)(\mu, j j) \), is positive. When \( c < 0 \), \( h(\mu)(\mu, j j) \) is negative. Such "anti-correlation" is seen between the fluctuations of the chiral condensate and the Polyakov loop in the results of lattice QCD calculations. The correlation between the variations of the two order parameters with respect to temperature is of the same sign as the correlation between the \( \mu \) fluctuations. Note that in the above Lagrangian when \( c = 0 \) the \( \mu \) field acts like an ordering field for the \( L \) field. In the chiral symmetry phase, the chiral order parameter is small and the Polyakov loop expectation value is zero. The large expectation value of \( L \) in the chiral symmetry phase, can result only from the last term in \( V(\mu; L) \) (with \( e > 0 \)) because \( j j \) is small.

As we have mentioned before, previous studies have considered only the interaction term \( g L^2 j j^2 \). When the coupling parameters \( c = 0 = e \), the chiral transition and the deconfinement transition do not always occur simultaneously. For large values of the coupling \( g \), the transitions can occur simultaneously and are of second order when coefficients of \( j j^2 \) and \( L^2 \) are negative in Eq. (1). A large positive \( g \) would increase the critical temperature for the deconfinement transition as the coefficient of \( L^2 \) term is negative for high temperatures. Lattice results on the other hand show that inclusion of dynamical quarks decreases the deconfinement transition temperature. So in QCD the coupling \( g \) should be small. For small \( g \) both the transitions are second order and do not occur simultaneously.

The coupling parameters \( c \) and \( e \) represent the strength of the \( Z_N \) explicit breaking. So they should increase with decreasing quark masses as the \( Z_N \) breaking becomes severe. This can be seen explicitly in the large quark mass region. To see the effect of the explicit \( Z_N \) breaking let us consider \( g = 0 = e \) and \( c \neq 0 \). At the mean-field level one can consider the temperature variation of the parameters \( m^2 \) and \( m_t^2 \). For simplicity we set \( m_t > 0 \), \( m_t^2 > 0 \) and vary the \( m^2 \) parameter. To understand the dependence of \( L \) and \( j j \) expectation values one has to solve the following coupled equations:

\[
\begin{align*}
    j j^3 + m^2 j j^2 &- 2cj L = 0 \\
    j L^3 + m_t^2 L &- cj j^2 = 0
\end{align*}
\]

We have checked numerically that for large enough \( c \) these equations give two solutions, which correspond to a degenerate minima of the effective potential \( V(\mu; L) \) at some particular value of \( m^2 \). It may seem surprising that the potential \( V(\mu; L) \) has degenerate minima even though there is no cubic term for \( j j \) and \( L \) in it. However, because of the coupling \( c \) these two minima are mixed. Though the mixing angle varies as \( m^2 \) is varied, with variation of \( m^2 \) the minima of \( V(\mu; L) \) in the \( j j \) and \( L \) plane, moves in directions other than the \( j j \) and \( L \) axes. To understand how the minima of \( V(\mu; L) \) vary one should express \( V(\mu; L) \) in terms of variables which are the linear combinations of \( j j \) and \( L \). This would invariably lead to cubic terms of the new fields in the effective potential. For some choice of parameters the cubic term may then be important to cause degenerate
Even if the explicit symmetry breaking is not strong enough at mean level, fluctuations at higher order can make the transition first order. At one loop the fluctuations of the field will contribute to a non-zero 3-point function of the L field. This 3-point function can be calculated perturbatively. In the high temperature approximation the 3-point function is given by,

$$\frac{T^3}{m^3};$$

assuming zero momentum to all the external L lines. m here is the mass of the field fluctuations. Given a suitable choice of parameters in the effective Lagrangian the three point function can be significant. The consequence of this is a $(\Gamma) L^3$ term in the potential $V(L)$ with temperature dependent $(\Gamma)$. This term can cause discontinuous change in L as temperature varies. When L field changes discontinuously the field will also change discontinuously because of the coupling term $c L^2$. If the coefficient of the $c L^2$ term changes from positive to negative due to discontinuous change in $L$ then will change discontinuously from zero to non-zero. The $L^3$ term can also come from other types of explicit symmetry breaking coupling terms but we think $c L^2$ is the simplest term in our model.

The situation with $c = 0$ and $g \neq 0 \neq e$ is same as the one discussed above. When the explicit symmetry breaking parameter is large, $Z_2$ symmetry of the L field is lost and the L field always has non-zero expectation value $L_0$. In order to study the fluctuations one must expand the potential $V(L)$ around $L_0$, $L = L_0 + \Delta L$. This gives rise to a term like $gL_0 L^2$ coming from the expansion of $gL^2$ around $L = L_0$. Now the term $gL_0 L^2$ is similar to the one discussed above. So there can be first order transition when $g \neq 0 \neq e$ like in the case when $c \neq 0$. We observed that at the mean field the transition becomes second order for large quartic couplings. Now in the following section we discuss the numerical Monte Carlo simulations of the effective Lagrangian (Eq. 1) and the results. These calculations include higher order as well as non-perturbative fluctuations.

### III. NUMERICAL CALCULATIONS AND RESULTS

The numerical Monte Carlo calculations of the model Eq. 1 is done by discretizing the action $S = \int d^3x$ on a 3 dimensional $N^3_s$ lattice. We employ the following rescaling of the fields variables and the couplings,

$$p \rightarrow \frac{p}{a} \; ; \; \; \; \; \; m \rightarrow \frac{m}{a^2} \; ; \; \; \; \; \; c \rightarrow \frac{c}{a^3} \; ; \; \; \; \; \; e \rightarrow \frac{e}{a^3}$$

$a$ is the lattice spacing and $L$ and $L'$ are the hopping parameters for the and the L field respectively. After the rescaling of the fields and the coupling parameters the discretized lattice
action becomes,

\[
S = \sum_{x} \left[ x \cdot x + \sum_{+} j \cdot \hat{\sigma} + (j \cdot \hat{\sigma} - 1)^2 \right] L_x L_{x+} + L_x^2 + 2 (L_x^2 - 1)^2 \]

\[
gL_x^2 \cdot j \cdot \hat{\sigma} \cdot cL_x \cdot j \cdot \hat{\sigma} \cdot cL_x \quad (4)
\]

Here \( x (L_x) \) represents the value of the \( L \) field at the lattice site \( x \). \( x + \) represents the six nearest-neighbor lattice sites to \( x \). We adopted the pseudo-heat-bath method used for the Higgs updating in SU(2)+Higgs studies \[13\]. To update \( x \) at a lattice site \( x \) we write the probability distribution \( P (x) \) of \( x \) as,

\[
P (x) = \text{Exp}[ S_1 (x) - S_2 (x)]; \quad \text{with} \]

\[
S_1 (x) = \sum_{+} A j^2 \quad ; \quad S_2 (x) = \sum_{+} j \cdot \hat{\sigma} \quad \text{B}^2
\]

\[
A = \sum_{+} X j \quad ; \quad B = 1 + \frac{1}{2} + \frac{cL_x + gL_x^2}{2} \quad (5)
\]

The coefficient \( A \) is a parameter chosen so that we get a reasonable acceptance rate for the new \( x \). Once chosen, a Gaussian random number is generated according to the distribution \( \text{Exp}[ S_1 (x)] \). Then this random number is accepted as the new value of \( x \) with the probability \( \text{Exp}[ S_2 (x)] \). Using this procedure, \( x \) is updated at all the lattice sites. Then we do the updating of \( L_x \) along the same steps. The process of updating \( x \) and \( L_x \) on the entire lattice is repeated about 20 times between successive measurements. We measure the magnetizations

\[
M = \frac{1}{V} \sum_{x} x \quad ; \quad M_L = \frac{1}{V} \sum_{x} L_x \quad (6)
\]

where \( V = N_x^3 \) is the number of lattice sites. The expectation values of the fields and the \( L_x \) fields are given by the thermal averages (average over the measurements), \( h_i = \frac{1}{M} \sum_{x} h_i \) and \( h_L = \frac{1}{M} \sum_{x} h_L \). We take the absolute value of \( M \) for \( h_i \) because a normal average of \( M \) is usually not a well-behaved observable.

The numerical simulations were carried out on a \( N_x = 16 \) lattice. In this work, we do not intend to explore the phase diagram of the model (Eq. 1) but to show that for suitable choice of parameters the phase transition can change from second order to first order. Here we present results for two sets of parameters. For one set we take the couplings \( g = e = 0 \) and for the second set we take the coupling \( c = 0 \). For the first set of parameters we choose, \( e = 0.004, \quad L = 0.0020, \quad L = 0.01 \) and \( c = 0.1 \). We observe the hysteresis of \( h_i \) and \( h_L \) by varying the parameter \( e \). In Fig. 1 we show the hysteresis loop of \( h_i \) and in Fig. 2 we show the hysteresis loop of \( h_L \).

Since we take \( c \) to be positive, we see \( h_i \) and \( h_L \) increase or decrease simultaneously. The choice of the values for the parameters is such that the variation of \( h_i \) and \( h_L \) are similar in magnitude. For \( c < 0 \) increase in \( h_i \) should lead to decrease in \( h_L \). So in this case the hysteresis loop for \( h_i \) will look somewhat similar to Fig. 1 while the hysteresis loop for \( h_L \) will be more or less inverted about the \( y \)-axis.

For the second set of parameters we choose, \( e = 0.0055, \quad L = 0.0010, \quad L = 0.14, \quad g = 0.02 \) and \( e = 0.9 \). The hysteresis loop of \( h_i \) and \( h_L \) are observed by again varying the parameter \( e \). The choice of \( L \) and \( e \) is such that the expectation value of \( L \) is non-zero and positive. The sign of \( g \)
assures that increase in $h_i$ leads to decrease in $hL_i$ and vice-versa as the parameter is varied. The hysteresis curves of the two order parameters are shown in FIG. 3 and FIG. 4. The values of $\mu$ in our calculations are chosen so that we can see 1st order phase transition clearly and the variation of $h_i$ and $hL_i$ are of order O (1) across the transition point. Note that with suitable choice of $L_i$ and $L_L$ one can change the average of the Polyakov loop across the transition point. The choice $g$ was such that the chiral transition turned out to be second order when the coupling $c$ was set to zero. We also did simulations on a 4D lattice. The results in this case are very similar to the 3D simulations.

The results in FIG. 1-4 show strong 1st order phase transition for the $h_i$ and $hL_i$ fields. By fixing the coupling parameters $g$, $c$, and $e$ we observed that the strength of the transition depends on the values of the quartic couplings $\mu$ and $\mu_L$. The transition becomes weaker with increase in any of the quartic couplings $\mu$, $\mu_L$. However even for larger quartic couplings a suitable choice of the parameters $g$, $c$, and $e$ made the transition strong 1st order.
We also did calculations with small explicit symmetry breaking for the field by considering a linear term in the Lagrangian. In this case we found that the hysteresis loops of both $h_i$ and $h_i$ shrinking in size with increase in the coset of linear term in the Lagrangian. These results suggest that the transition becomes weaker when the chiral symmetry is explicitly broken.

IV. DISCUSSION AND CONCLUSIONS

Using a simple effective Lagrangian, which captures the chiral symmetry and $Z_N$ symmetry of QCD, we have investigated the effect of the explicit symmetry breaking on the chiral phase transition. Since we consider the chiral limit of the $Z_2$ symmetry of the Polyakov loop is explicitly broken. As we incorporate the explicit $Z_2$ breaking interaction terms in the effective Lagrangian we find the chiral transition becomes first order. We observed that the first order transition becomes weaker when a small explicit symmetry breaking is considered for the chiral order parameter. The results of our calculations show that two flavor chiral transition is of first order for large enough $Z_N$ explicit breaking. As we have mentioned before at present some lattice studies suggest that the transition is second order and some other studies show the transition is second order. These conflicting results may be because the quark mass studied are not small enough or the lattices used are not big enough.

In the previous study, for $N_f = 2$ and $N = 3$, the second order chiral transition becomes first order when coupled to the Polyakov loop. This is because the deconfinement transition is first order for $N = 3$ with a cubic term $(L^3 + L^3)$ in the effective potential with exact $Z_3$ symmetry. However, when the quark masses are small and decrease the deconfinement transition becomes weaker. This can be understood due to explicit breaking of $Z_3$ symmetry. A ready in the large quark mass region the deconfinement transition becomes crossover which implies the the explicit symmetry breaking dominates over the effects of the above $Z_3$ symmetric cubic term. For smaller quark mass the explicit $Z_3$ symmetry breaking likely grows and expected to be maximal in the chiral limit. So for smaller quark masses, i.e. in the chiral limit, one should rather consider the effect of the explicit breaking of the $Z_3$ symmetry. The effects of explicit symmetry breaking discussed in this work should not be restricted to the explicit breaking of the $Z_N$ symmetry. For 2-flavor and 2-color QCD the deconfinement transition in the large quark mass region may have the effects coming from the explicit breaking of the chiral symmetry. It may be possible that this effect change the phase transition behavior of the deconfinement transition in the heavy quark mass region.

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