Diquark Condensation at Nonzero Chemical Potential and Temperature

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Abstract

$SU(2)$ lattice gauge theory with four flavors of quarks is studied at nonzero chemical potential $\mu$ and temperature $T$ by computer simulation and Effective Lagrangian techniques. Simulations are done on $8^4$, $8^3 \times 4$ and $12^3 \times 6$ lattices and the diquark condensate, chiral order parameter, Wilson line, fermion energy and number densities are measured. Simulations at a fixed, nonzero quark mass provide evidence for a tricritical point in the $\mu$-$T$ plane associated with diquark condensation. For low $T$, increasing $\mu$ takes the system through a line of second order phase transitions to a diquark condensed phase. Increasing $T$ at high $\mu$, the system passes through a line of first order transitions from the diquark phase to the quark-gluon plasma phase. Using Effective Lagrangians we estimate the position of the tricritical point and ascribe its existence to trilinear couplings that increase with $\mu$ and $T$.

12.38.Mh, 12.38.Gc, 11.15.Ha
Recently there has been a resurgence of interest in QCD at nonzero chemical potential for quark number. Arguments based on instantons and phenomenological gap equations support the old idea that diquark condensation and a color superconductivity phase transition will occur at a critical chemical potential of slightly less than one-third the proton’s mass. Unfortunately, some of these arguments and calculations could prove to be misleading because a proper understanding of the diquark state alludes the field: since diquarks carry color in real QCD, a quantitative understanding of confinement and screening is needed to estimate the energies of the states which control the phases of the system. In addition, the brute force lattice simulation method does not yet have a reliable simulation algorithm for these environments in which the fermion determinant becomes complex.

Since true QCD at finite quark-number chemical potential cannot be simulated with current methods, theorists have turned to simpler models which can be simulated. One of the more interesting is the color SU(2) version of QCD which addresses some of the issues of interest. In this model diquarks do not carry color, so their condensation does not break color symmetry dynamically. The critical chemical potential is also expected to be one-half the mass of the lightest meson, the pion, because quarks and anti-quarks reside in equivalent representations of the SU(2) color group. Chiral Lagrangians can be used to study the diquark condensation transition in this model because the critical chemical potential vanishes in the chiral limit, and the model has a Goldstone realization of the spontaneously broken quark-number symmetry. Lattice simulations of the model are also possible because the fermion determinant is non-negative for all chemical potentials. One hopes that these developments will uncover generic phenomena that will also apply to QCD at nonzero chemical potential.

Preliminary lattice simulations of the SU(2) model with four species of quarks have been presented at conferences recently, and it is the purpose of this article to present the continuation of that work with a focus on the system’s phase diagram at nonzero $\mu$ and $T$. Earlier work on this model at finite $T$ and $\mu$ was performed by More detailed discussion of our zero temperature, finite $\mu$ simulations including the spectroscopy of the
light bosonic modes will be presented elsewhere [7]. We choose to consider the system’s phase diagram here because of its elementary, fundamental character and because these simulations produced an unanticipated result compared to what has been found previously in various models [8,9]. For fixed quark mass, which insures us that the pion has a nonzero mass and chiral symmetry is explicitly broken, we find a line of transitions separating a phase with no diquark condensation from one with a diquark condensate. Along this line there is a tricritical point where the transition switches from being second order (and well described by mean field theory) at relatively low \( \mu \) to a first order transition at an intermediate \( \mu \) value. At large \( \mu \) the line of first order transitions separates the diquark condensate phase at low \( T \) from a quark-gluon phase at high \( T \). The transition is clear in diquark observables as well as the Wilson Line. A schematic phase diagram is shown in Fig.1. (Note that we have not included the line of first order transitions starting from the \( \mu = 0 \), finite temperature transition, which exists for \( m \) small enough). We shall see that this simulation result, the existence of a tricritical point, has a natural explanation in the context of chiral Lagrangians. Following the formalism of [10] we shall argue that trilinear couplings among the low lying boson fields of the Lagrangian become more significant as \( \mu \) and \( T \) increase and they can cause the transition to become first order at a \( \mu \) value in the vicinity of the results found in the simulation. By hindsight, this behaviour should not have come as a surprise. \( \mu \) plays the rôle of a second ‘temperature’ in this theory in that it is a parameter that controls diquark condensation, but does not explicitly break the (quark-number) symmetry. The existence of two competing ‘temperatures’ is a characteristic of systems which exhibit tricritical behaviour.
FIG. 1. Schematic Phase Diagram in the $T$-$\mu$ Plane. The thin(thick) line consists of second(first) order transitions. X labels the tricritical point.

We begin with a discussion of the simulation method and the numerical results.

The lattice action of the staggered fermion version of this theory is:

$$S_f = \sum_{\text{sites}} \left\{ \bar{\chi} [\mathcal{D}(\mu) + m] \chi + \frac{1}{2} \lambda \left( \chi^T \tau_2 \chi + \bar{\chi} \tau_2 \bar{\chi}^T \right) \right\}$$

(1)

where the chemical potential $\mu$ is introduced by multiplying links in the $+t$ direction by $e^\mu$ and those in the $-t$ direction by $e^{-\mu}$. The diquark source term (Majorana mass term) is added to allow us to observe spontaneous breakdown of quark-number on a finite lattice. The parameter $\lambda$ and the usual mass term $m$ control the amount of explicit symmetry breaking in the lattice action. We will be particularly interested in extrapolations to $\lambda \to 0$ for a given $m$ to produce an interesting, realistic physical situation. This is the case that has been studied analytically using effective Lagrangians at vanishing temperature $T$ but nonvanishing chemical potential $\mu$.\[11\], \[12\].

Integrating out the fermion fields in Eq.1 gives:

$$\text{pfaffian} \begin{pmatrix} \lambda \tau_2 & A \\ -A^T & \lambda \tau_2 \end{pmatrix} = \sqrt{\det(A^\dagger A + \lambda^2)}$$

(2)

where
\[ \mathcal{A} \equiv \mathcal{D}(\mu) + m \]  

(3)

Note that the pfaffian is strictly positive, so that we can use the hybrid molecular dynamics [13] method to simulate this theory using “noisy” fermions to take the square root, giving \( N_f = 4 \).

For \( \lambda = 0, m \neq 0, \mu \neq 0 \) we expect no spontaneous symmetry breaking for small \( \mu \). For \( \mu \) large enough \( (\mu > m_\pi/2 \) according to most approaches including Chiral Perturbation Theory [10], [12]) we expect spontaneous breakdown of quark number and one Goldstone boson – a scalar diquark. (The reader should consult [4] for a full discussion of the symmetries of the lattice action, remarks about spectroscopy, Goldstone as well as pseudo-Goldstone bosons, and for early simulations of the 8 flavour theory at \( \lambda = 0 \).)

Now consider the simulation results for the \( N_f = 4 \) theory on \( 8^4, 8^3 \times 4 \) and \( 12^3 \times 6 \) lattices, measuring the chiral and diquark condensates \( \langle \chi^T \tau_2 \chi \rangle \), the fermion number density, the Wilson/Polyakov line, etc. We are also engaged in larger scale simulations on \( 12^3 \times 24 \) lattices, where, in addition, we are measuring all local scalar and pseudoscalar meson and diquark propagators (connected and disconnected). These simulations will be presented in our paper on zero temperature results [7]. Some of these results, especially for relatively large quark mass have been previewed elsewhere [5].

First consider measurements on a \( 8^4 \), 'zero temperature' lattice. We simulated the \( SU(2) \) model at a relatively strong coupling \( \beta = 1.0 \) to avoid finite size and temperature effects. (More extensive simulations at \( \beta = 1.5 \) and \( m = 0.1 \) also on an \( 8^4 \) lattice will be presented in our zero temperature paper.) The quark mass was \( m = 0.05 \) and a series of simulations were done at \( \lambda = 0.0025, 0.005, \) and \( 0.01 \) so that our results could be extrapolated to vanishing diquark source, \( \lambda = 0 \). Simple linear and spline extrapolations were done and these procedures appeared to be sensible for these exploratory calculations. In the future more theoretical control over the \( \lambda \to 0 \) limit will have to be developed. None of the conclusions to be drawn here will depend strongly on the limit. In fact, everything we say could be gathered from our data at a fixed (small) \( \lambda \) value, 0.005 say. However, only in the
limit of vanishing $\lambda$ do we expect real diquark phase transitions (at least when the transitions are second order), so it is interesting and relevant to begin investigating the $\lambda \to 0$ limit.

Two further difficulties occur for small $\lambda$. First, the Hybrid algorithm slows down as $\lambda$ is taken small and diquark observables are calculated. Analogous problems are familiar in QCD simulations at vanishing $\mu$ but small $m$ because the Dirac operator of the standard lattice action becomes singular in the chiral limit [13]. Even these exploratory simulations are quite CPU intensive for this reason, although they are well within the capabilities of standard PC’s, and workstations. (Most of the results reported here were done on SV1 workstations at NERSC and the T90 vector processor at NPACI.) Second, the Hybrid algorithm suffers from systematic errors proportional to the discrete time step used in integrating its stochastic differential equations forward in Monte Carlo time [13]. Most of the simulations reported here used a time step $dt = 0.005$ to control these errors. Future, accurate simulations on larger lattices will need even smaller time steps. $dt = 0.005$ proved adequate here but systematic errors are under investigation and will be reported on at a later date.

In Fig.2 we show the diquark condensate plotted against the coupling $\beta$. The quark mass $m$ was set at 0.05, the coupling was $\beta = 1.0$ and $\lambda$ has been extrapolated to zero using raw data at $\lambda = 0.0025$ and 0.005.

![Diquark Condensate vs. $\mu$](image)

**FIG. 2.** Diquark Condensate vs. $\mu$
We see good evidence to a quark-number violating second order phase transition in this figure. The dashed line is a power law fit which picks out the critical chemical potential of \( \mu_c = 0.2573(2) \). Since the coupling here is too large to reside in the gauge theory’s scaling window and the lattice is too small to escape significant coarse-grain errors, we expect only semi-quantitative results. However, the power law fit is fair, its confidence level is 7 percent, and its critical index is \( \beta_{\text{mag}} = 0.32(5) \) which is somewhat smaller than the mean field result \( \beta_{\text{mag}} = 1/2 \), predicted by lowest order chiral perturbation theory \cite{10}, \cite{12}. Note that the quark mass is fixed at \( m = 0.05 \) throughout this simulation, so chiral symmetry is explicitly broken and this transition is due to quark number breaking alone. In fact, the chiral order parameter \( \langle \bar{\chi}\chi \rangle \) is nonzero and varies smoothly from 1.00 to 0.50 over the critical region shown in Fig. 2. The fermion number density, shown in Fig. 3, also shows the diquark continuous phase transition. The approximate linear dependence of the fermion number density with \( \mu \) is the expected scaling behavior above the transition in lowest order chiral perturbation theory \cite{10}, \cite{12}.

![FIG. 3. Fermion Number Density vs. \( \mu \)](image)

Now we turn to the main focus of this letter, the phase diagram in the temperature-chemical potential plane. To begin, consider the small \((8^3 \times 4)\) lattice results.
Consider a slice through the phase diagram at a fixed small temperature, for variable $\mu$. In Fig.4 we show the diquark condensate for $\beta = 1.3$, $m = 0.05$, with the data extrapolated to $\lambda = 0$ as discussed above. As $\mu$ increases we find that a second order phase transition to a diquark condensate appears at $\mu_c = 0.2919(4)$. The dashed line fit in Fig.4 has the critical index $\beta_{mag} = 0.50(15)$, in good agreement with mean field theory. The fit has a confidence level of 21 percent. The diquark transition is also clear in a plot of the fermion number density, as expected. However, the chiral condensate varies smoothly over the diquark critical region, with $\langle \bar{\chi} \chi \rangle$ ranging from 0.80 to 0.50. The Wilson Line is also smooth, varying from 0.10 to 0.20, with no obvious signs of a transition.

Simulations at $\beta = 1.1$ and 1.5 gave similar conclusions. At $\beta = 1.1$, there was a continuous diquark transition at $\mu = 0.2544(3)$ and at $\beta = 1.5$ there was a continuous diquark transition at $\mu = 0.2950(3)$. So, as the system is heated ($\beta$ increases), a larger chemical potential is needed to order the system into a diquark condensate.

Next, simulations were run at fixed $\mu$ and variable $\beta$. First, consider a relatively large and interesting $\mu = 0.40$. We show the diquark condensate as a function of $\beta$ for $\mu = 0.40$ in Fig.5. There is a clear jump in the condensate at $\beta = 1.55(5)$, suggesting a first order
phase transition.

A discontinuous transition is also strongly suggested by the behavior of the Wilson Line shown in Fig.6.

If this transition at relatively large \( \mu \) and \( T \) is really first order, then there should be a tricritical point separating the region of continuous transitions at smaller \( \mu \) and \( T \). We
strengthened the evidence for a first order transition at $\mu = 0.40$ by running the algorithm on a larger $(12^3 \times 6)$ lattice. In Fig. 7, 8, and 9 we show the diquark condensate, the Wilson line and the chiral condensate on the $12^3 \times 6$ lattice.

**FIG. 7.** Diquark Condensate vs. $\beta$.

**FIG. 8.** Wilson Line vs. $\beta$. 

![Graph of diquark condensate vs. beta](image-url)

![Graph of Wilson line vs. beta](image-url)
In all figures we see evidence for a discontinuous transition at $\beta = 1.97(2)$ separating a diquark condensate and a quark-gluon plasma phase. Note that these are figures of raw data are taken at $\lambda = 0.005$. However, since the transition appears first order, it should extend to finite (although probably small) $\lambda$.

$\beta = 1.97(2)$ lies in the scaling window of the $SU(2)$ lattice gauge theory with four species of dynamical quarks, so we can compare our $\mu_c = 0.40$ to the theory’s spectroscopic mass scales [14]. In fact, $m_\pi/2 = 0.31(1)$, so finite $T$ effects have apparently raised $\mu_c$ somewhat from its zero $T$ value, $m_\pi/2$. Such effects will be discussed below in the context of Effective Lagrangians.

The exact location of the tricritical point should be found in larger scale simulations. On our small $8^3 \times 4$ lattices we have some evidence that it lies between $\mu = 0.30$ and 0.40. In particular, we repeated the simulations that produced the data in Fig.’s 5 and 6, but at $\mu = 0.30$ and produced Fig.’s 10 and 11.
The dashed curve in Fig.10 is a power law fit to the data which has a confidence level of 15 percent, a critical index $\beta_{mag} = 0.59(15)$ and critical coupling $\beta_c = 1.4740(5)$. According to lowest order chiral perturbation theory, the critical behavior along the entire line below the tricritical point should be in one Universality Class, Mean Field Theory, while a tricritical point should have distinct indices, including $\beta_{mag}^{tri} = 1/4$. It would be challenging
and particularly interesting to confirm the value $\beta_{mag}^{\text{tri}} = 1/4$ in the next round of lattice simulations, on larger lattices closer to the theory’s continuum limit.

Is this tricritical point suggested here expected theoretically? To answer this question we studied the possibility of a first order phase transition between the superfluid and the normal phases using the Landau approach. Our goal was to analytically understand the emergence of the first order phase transition observed in the numerical simulations at high enough $\mu$, not to describe the second order phase transition for chemical potentials just above $\mu_c = m_\pi/2$. We constructed the Landau free energy that describes the behavior of the diquark condensate for chemical potential greater than $\mu_c$. Within this approach there is indeed a first order phase transition that separates the superfluid and the normal phases for high enough $\mu$.

In order to construct the Landau free energy, we have first to determine the symmetries of the system [15]. The low-energy effective Lagrangian that has been used to describe QCD with two colors and quarks in the fundamental representation at zero temperature and nonzero chemical potential in [10,12] is solely based on the symmetries of the QCD partition function. For small enough temperatures, the symmetries remain the same as at $T = 0$. Therefore the effective Lagrangian provides us with a natural basis to investigate the symmetries of the system in the superfluid phase at nonzero temperature. We only need to use the substantial properties of the low-energy effective Lagrangian. The reader is invited to consult [10,12] for a more detailed discussion of the effective Lagrangian itself. The effective Lagrangian at lowest order reads

$$\mathcal{L}_{\text{eff}} = F_\pi^2 \left[ \frac{1}{2} \text{Tr} \partial_\nu \Sigma^\dagger \partial_\nu \Sigma + 2\mu \text{Tr} B \Sigma^\dagger \partial_\nu \Sigma - \mu^2 \text{Tr} \left( \Sigma B^T \Sigma^\dagger + BB \right) - m_\pi^2 \text{Re} \text{Tr} \hat{M} \Sigma \right],$$

where $F_\pi$ is the pion decay constant, and $m_\pi$ is the pion mass. The matrix $B$ retains the symmetries of the chemical potential term in the QCD Lagrangian, and the matrix $\hat{M}$ retains the symmetries of the mass matrix. Finally the field $\Sigma = U\hat{\Sigma}U^T$ contains both the minimum $\hat{\Sigma}$ of (4) and the fluctuations around it, i.e. the Goldstone fields, $U = \exp(i\pi a T_a/F_\pi) \left( T_a \right)$.
are the generators of the Goldstone manifold). At $T = 0$ when $\mu$ reaches $\mu_c = m_\pi/2$, the minimum begins to rotate: $\bar{\Sigma} = \cos \alpha \Sigma_c + \sin \alpha \Sigma_d$, where $\Sigma_c$ corresponds to the quark-antiquark condensate, and $\Sigma_d$ corresponds to the diquark condensate. The angle of rotation is given by $\alpha = 0$ for $\mu < \mu_c$, and by $\cos \alpha = m_\pi^2/4\mu^2$ for $\mu > \mu_c$ \cite{10,12}. For $\mu > \mu_c$ the ground state of the system is a diquark condensation phase. The diquark condensate breaks the symmetry generated by the $U(1)$ baryon charge.

In the superfluid phase ($\mu > \mu_c$) and at zero temperature, if we expand the effective Lagrangian (4) in the fluctuations of $\Sigma$ (i.e. in the Goldstone fields), we find that there are terms that are even in the Goldstone fields, and that there are terms that are odd in the Goldstone fields. These odd terms come from the linear derivative term in (4); they are absent in the normal phase. These odd terms are always present in the superfluid phase, even at small temperature. They involve the long range excitations that carry the same quantum number as the diquark condensate. Hence the Landau free energy can be written as \cite{13}

$$L = A t \chi^2 + B \chi^3 + C \chi^4, \quad (5)$$

where $\chi$ is the order parameter, and $t = T/T_c - 1$ is the reduced temperature. The order parameter of the superfluid phase is the diquark condensate. The Landau free energy contains odd terms. They are not excluded by the symmetries of the system: as we saw above in the effective Lagrangian, these symmetries allow the presence of odd terms in the Goldstone fields that carry the same quantum numbers as the diquark condensate. This is very different from the situation at $\mu = 0$ where the symmetry excludes odd terms in the pion fields both for three colors and for two colors \cite{13,17}. From standard studies of critical phenomena, these odd terms are known to be able to drive a first order phase transition. We have expanded $L$ to $O(\chi^4)$ assuming that all the essential physics near the critical temperature $T_c$ appears at this order. Since $\chi = 0$ in the symmetric phase above the critical temperature, there cannot be any linear term in $\chi$, the coefficient of the quadratic term must be proportional to $t$, and $A$ has to be positive. Furthermore $C$ has to be positive so
that \(|\chi| \to \infty\) is not a minimum of the Landau free energy.

Some properties of the coefficients \(A, B,\) and \(C\) in (3) can be deduced from the effective Lagrangian (4). Once we are in the superfluid phase, the pion mass is practically irrelevant. For chemical potentials not very far above \(\mu_c\), the orientation of the condensate is almost completely in the diquark direction. From the effective Lagrangian (4) expanded to fourth order in the Goldstone fields and neglecting the pion mass, we infer that the coefficient in the Landau free energy (3) are of the following form

\[
A = a \mu^2, \quad a > 0 \\
B = b \mu(t+1) \\
C = c \mu^2/F_\pi^2, \quad c > 0.
\]

The temperature dependence of the coefficient of the cubic term \(B\) comes from the \(\partial_0 \Sigma\) term in the effective Lagrangian (4). This coefficient \(B\) has to vanish at zero temperature. Finally we get that the Landau free energy density is given by

\[
L = a t \mu^2 \chi^2 + b \mu(t+1) \chi^3 + c \frac{\mu^2}{F_\pi^2} \chi^4.
\]

Since we neglected the pion mass, the chemical potential we are using here has to be understood as \(\mu - \mu_c = \mu - m_\pi/2\). The Landau free energy (4) can only be used to describe the transition from the superfluid phase to the normal phase. Therefore the Landau free energy (7) is only valid for \(\mu > \mu_c\). For \(\mu - \mu_c \geq \mu_t = b F_\pi/\sqrt{ac}\), if \(t < (\mu_t/(\mu - \mu_c + \sqrt{(\mu - \mu_c)^2 - \mu_t^2}))^2\) the minimum is at \(\chi \neq 0\), but for \(t > (\mu_t/(\mu - \mu_c + \sqrt{(\mu - \mu_c)^2 - \mu_t^2}))^2\), the minimum jumps to \(\chi = 0\). The Landau free energy (7) therefore predicts a first order phase transition for \(\mu > \mu_c + b F_\pi/\sqrt{ac}\). For \(\mu - \mu_c < \mu_t\) the cubic term cannot drive a first order transition. From this analysis we thus expect that for \(\mu - m_\pi/2\) of the order of \(F_\pi\) a first order phase transition separates the superfluid phase from the normal phase.

At \(T = 0\) a second order phase transition separates the superfluid and the normal phases. From continuity arguments, the phase transition between these two phase has to remain second order for small enough temperatures. With the arguments given above, we
find that the phase transition is going to become first order above some chemical potential. We therefore find that there is a tricritical point in the phase diagram. Our analysis is too crude to tell the exact position of the tricritical point, but it predicts that it should correspond to $\mu - m_\pi/2$ of the order of $F_\pi$.

This work will be followed up by several additional investigations. We certainly need to improve the numerical data by running on larger lattices, closer to the theory’s continuum limit. Once that is done and more spectroscopy data is accumulated, we will be able to state our results in physical units and check many of the predictions of lowest order chiral perturbation theory quantitatively. It will also be interesting to study QCD with small chemical potentials associated with the three light quark flavors [18], [19]. In particular, we expect the phase diagram at nonzero isospin chemical potential and temperature to be very similar to the one discussed here. Although we cannot attack the SU(3) theory with a large Baryon number chemical potential, these other situations can be studied both analytically and numerically, and interesting new phases of matter have been found there which should be investigated further.

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