New possibilities for QCD at finite density

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I review the growing theoretical indications that at high densities color SU(3) gauge symmetry is spontaneously broken by the formation of a quark pair condensate. This leads to a rich phase structure for QCD as a function of temperature and chemical potential.

I also discuss the prospects for lattice QCD calculations at finite density, including the Glasgow algorithm and imaginary chemical potential.

1. Superconducting phases of QCD

The behavior of matter at high quark density is interesting in itself and is relevant to phenomena in the early universe, in neutron stars, and in heavy-ion collisions. Recent analyses of Nambu–Jona-Lasinio (NJL) models of high-density QCD, in which the gluons are replaced by a four-fermion interaction, indicate interesting physics. In particular, exotic superconducting phases may occur above nuclear density. Both two- and three-flavor cases have been studied, and I will discuss them in turn, before going on to the topic of lattice techniques.

1.1. Two-flavor QCD

Figure 1 gives a plausible phase diagram for QCD with two massless flavors. The main division is into chirally broken and symmetric phases: axial flavor is broken at low temperatures/densities, and restored at high ones. For a very clear discussion and further references see Ref. [1]. The chiral phase transition is believed to be second order at $\mu = 0$, and the indications from bag and matrix models are that it is first order at $T = 0$. Thus there is a tricritical point (solid circle) at the switch-over from second order to first order [2]. In the low-temperature chirally broken region there is the nuclear gas-liquid phase transition line, which ends at a critical point (empty circle) at $T \sim 10$ MeV.

At low temperatures, it is becoming clear that additional interesting phases occur above the chiral-symmetry-restoring chemical potential. It was originally suggested by Bailin and Love [3] (see also [4]) that QCD at high density might behave analogously to a superconductor: through the BCS mechanism [5], Cooper pairs of quarks condense in an attractive channel, breaking the color gauge symmetry, and opening a gap at the Fermi surface. Recent mean-field/variational analyses of NJL models of QCD, using the 4-leg instanton vertex as the effective interaction [6,7], indicate that BCS-style quark pair condensation does indeed occur, and that the gaps are phenomenologically significant—of order 100 MeV—at densities only a few times nuclear density. The simplest form of pairing is a spin (indices suppressed) and flavor (indices $i, j$) singlet, which by antisymmetry of the fermion wavefunctions must form a color $3\bar{3}$ (indices $\alpha, \beta$):

$$\langle S | q^\alpha_i C \gamma^5 q^\beta_j | S \rangle \propto \epsilon_{ij} \epsilon^{\alpha\beta},$$

(1)

The coherent state $|S\rangle$, consisting of a quark pair condensate, has lower free energy than the perturbative vacuum, indicating that in the true vacuum two quark colors (red and green, say) condense, leaving the blue quarks forming a Fermi surface.

In QCD, unlike the NJL model, color is a gauged symmetry, so there is no local order parameter to distinguish the superconducting phase of QCD from the deconfined one. As in the standard model, however, we expect there to be a first-order phase transition or crossover between regions of parameter space with quite different
physics. The equation of state, according to NJL models, is only slightly affected by quark pair condensation. The two main features that characterize the superconducting phase are (1) There is a gap in the fermion spectrum. (2) The condensate changes the electric charges of the quarks, since it breaks color and electromagnetism down to color $SU(2)$ and a new electromagnetism that is a combination of the photon and one of the gluons.

It would be very useful to translate these into some observable for heavy ion collisions, but this has not yet been done.

At very low temperatures, a more exotic phase may form. The blue quarks, left out of the superconducting condensate, may form spin-1 pairs and condense, breaking rotational invariance and the remaining $SU(2) \times U(1)_{em}$ gauge symmetry. NJL calculations indicate a parameter-sensitive and small gap ($\sim 1$ keV) in this channel, leaving open the intriguing possibility that such a phase might play a role in neutron stars.

1.2. Three-flavor QCD

Fig. 2 shows a conjectured phase diagram for QCD with 3 massless flavors. We have to use the single-gluon-exchange vertex as the effective interaction, since the instanton vertex now has an odd number of quark legs, and cannot be saturated by a quark pair condensate. However, now that the number of flavors and colors is the same, a different form of condensate is possible:

$$\langle S | q_1^\alpha \bar{q}_1 C^\gamma \gamma_5 q_2^\beta | S \rangle = \kappa_1 \delta_1^\alpha \delta_2^\beta + \kappa_2 \delta_1^\beta \delta_2^\alpha ,$$

(2)

The mixed Kronecker $\delta$ matrices are invariant under correlated vectorial color/flavor rotations (“color-flavor locking”). The breaking pattern is $SU(3)_{color} \times SU(3)_L \times SU(3)_R \times U(1)_{B} \rightarrow SU(3)_{diag}$, where $SU(3)_{diag}$ is the diagonal SU(3) subgroup of the first three factors. The color symmetry (gauged in QCD) is broken by the
quark pair condensate, but, unlike the two-flavor case, chiral symmetry is also broken. Also, with 3 flavors there is a gauge-invariant order parameter, corresponding to the breaking of baryon number: \( \langle NN \rangle \).

1.3. Generalities

The detailed NJL-model calculations that show quark pair condensation are given in \[6–8\]. Nambu and Jona-Lasinio explicitly based their studies of chiral symmetry breaking on BCS, and described the chiral condensate as a "superconductive' solution" \[9\]. However, there are important differences (Fig. 3). Chiral symmetry breaking is caused by a condensate of particle-antiparticle pairs with zero net momentum. In the presence of a Fermi surface with Fermi momentum \( p_F \), one can only create particles with \( p > p_F \), so as the density grows, more and more states are excluded from pairing, and chiral symmetry breaking is suppressed. In contrast, color symmetry breaking involves pairs of particles or pairs of antiparticles. Near the Fermi surface these pairs can be created at negligible cost in free energy, and so any attractive particle-particle interaction enables the pairs to lower the free energy. This is the BCS instability of the perturbative vacuum. If there is any channel in which the interaction between quarks is attractive, then quark pair condensation in that channel will occur. As density increases, the phase space available near the Fermi surface grows, and more quark pairing occurs.

There are many directions in which to continue investigating quark pair condensates: experimental signatures in heavy ion collisions, their possible role in neutron star physics, and of course the 2+1 flavor case, with a realistic strange quark mass.

Finally, it would be valuable to perform lattice calculations of the finite density behavior of both the toy models and QCD. Hands and Morrison \[10\] have performed lattice simulations of a Gross-Neveu model, which is very similar to the NJL model used here, but they have not yet seen unambiguous evidence of quark pairing. Finite density calculations in QCD, however, remain a much more elusive goal. This is the topic of the rest of this paper.

2. Lattice QCD at finite density

The usual approach to fermions is to integrate them out:

\[
Z(\mu) = \sum_N Z_N e^{-\mu N} = \sum_{U(x)} \frac{\text{det} M e^{-S_{\text{glue}}[U]}}{S_{\text{ferm}}} \quad \text{sampling weight} \quad (3)
\]

\[
S_{\text{ferm}} = \int_x \bar{\psi} M \psi
\]

For Monte Carlo evaluation, the sampling weight must be positive, so \( \text{det} M \) must be non-negative for any gauge configuration. One way to guarantee this is if we have an even number of flavors, each with the same fermion matrix \( M \), and \( M \) is similar to its adjoint, so the eigenvalues are real or in complex-conjugate pairs, and \( \text{det} M \in \mathbb{R} \).

\[
M^\dagger = PMP^{-1} \quad \text{for some } P, \quad N_F \text{ even} \quad (4)
\]

This is the situation in zero-density lattice QCD. For the Wilson action, for example,

\[
M = \gamma^\mu D_\mu + r D^2 + m + \mu \gamma_0
\]

\[
M^\dagger = -\gamma^\mu D_\mu + r D^2 + m + \mu \gamma_0 \quad (5)
\]
so without a chemical potential (4) is obeyed with $P = \gamma_5$, but introducing a real chemical potential violates this condition. $\det M$ is then complex, and straightforward Monte-Carlo methods are inapplicable. Similar conclusions obtain for Kogut-Susskind quarks. This is the “sign problem”, which is really a phase problem for QCD. It is interesting to note, however, that an imaginary chemical potential leaves the measure positive.

2.1. The Glasgow method

For the last decade, the approach to finite density QCD that has been most seriously pursued is the Glasgow method, [11,12]. This avoids the positivity problem by treating the chemical potential analytically: $Z$ is expanded in powers of the fugacity $e^{\beta\mu}$, and the coefficients are evaluated by Monte-Carlo using the $\mu = 0$ weighted ensemble.

$$Z(\mu) = \left\langle \frac{\det M(\mu)}{\det M(0)} \right\rangle_{\mu=0}$$

Unfortunately, the Glasgow method does not reproduce the most fundamental property expected of QCD at finite chemical potential, namely the onset of baryon density when $\mu$ reaches $M_{\text{baryon}}/3$. Instead, the onset seems to begin at a lower chemical potential $\mu_o \sim M_\pi/2$. This is the behavior of the quenched theory, in which there is an unphysical baryonic pion state [13].

In the last year, there has been a convergence of opinion that the Glasgow method will eventually show the correct onset behavior, but only at very large statistics. This is because of the “overlap problem”, a mismatch between the regions of configuration space that are emphasized by the $\mu = 0$ ensemble, and the regions that are relevant for the finite-density physics. Because of the measure mismatch, the integral comes from large but rare fluctuations in the reweighting factor in (6), making it necessary to accumulate a huge number of configurations.

The evidence for this conclusion has come from several sources. (1) Using the Glasgow method for QCD on a tiny $2^4$ lattice, Barbour [15] finds that $\mu_o$ rises towards $m_N/3$ at very high statistics. (2) The Gross-Neveu model has been studied in 2+1 dimensions [3]. It has quarks and conjugate quarks, so there is no sign problem, and one can perform updates at any chemical potential. At moderate statistics, the onset behavior shows dependence on the value of $\mu$ used in the updating (see Fig. 4). (3) Azcoiti et al [16] argue that the phase of the quark determinant drops as $\exp(-V)$, so statistics $\sim \exp(V)$ is needed. (4) Halasz [17] has studied matrix models of the QCD fermion determinant, and finds that they need statistics $\sim \exp(N)$.

2.2. Imaginary chemical potential

As was noted above, with imaginary chemical potential $\mu = i\nu$, $\det M$ is real, and the functional integral can be evaluated by standard Monte-Carlo methods [18–20]. We still have to choose an updating value $\nu_{\text{update}}$, and then “reweight” to obtain $Z(i\nu)$, but the reweighting factor is always positive, so there is no phase problem, and very

![Figure 4. Fermion density as a function of chemical potential $\mu$ for the Gross-Neveu model [14], calculated from moderate statistics using Glasgow reweighting of ensembles generated at chemical potentials $\mu_{\text{update}} = 0.0, 0.7, 0.8$, as well as the exact (unreweighted) result. Note how the apparent onset depends on $\mu_{\text{update}}$, indicating that the $\mu_{\text{update}} = 0$ ensemble used for QCD may give unreliable results at moderate statistics.](image-url)
high statistics is not needed.

\[
\frac{Z(i\nu)}{Z(i\nu_{\text{update}})} = \left\langle \frac{\det M(i\nu)}{\det M(i\nu_{\text{update}})} \right\rangle_{\mu=i\nu_{\text{update}}}.
\]  

(7)

We can cover \(\nu = 0 \ldots 2\pi/\beta\) with “patches” centered at several different \(\nu_{\text{update}}\), and thereby ensure that the reweighting factor has arbitrarily small fluctuations. Then we must Fourier transform to get canonical partition functions

\[
Z_N = \frac{\beta}{2\pi} \int_{0}^{2\pi/\beta} d\nu \, Z(i\nu) e^{-i\beta\nu N}.
\]  

(8)

The Fourier transform is the place where large errors may arise. Imaginary chemical potential does not bias the ensemble towards states with higher quark number; it relies on thermal or quantum fluctuations to supply such states, and it gives them a characteristic weighting. If such fluctuations are too rare then \(Z(i\nu)\) will be dominated by \(Z_0\), and very large statistics will be needed to see the effects of the higher \(Z_N\). This is not necessarily a problem: as the temperature \(T\) rises towards the deconfining phase transition \(T_c\), the baryon becomes lighter, so \(M_B/T\) may become small enough for thermal fluctuations to populate the system with baryons. Calculating the \(Z_N\) by \(\left\langle \right\rangle\) will then be straightforward. The Glasgow algorithm may also be expected to work better as \(T \to T_c\).

2.3. The Hubbard model with imaginary \(\mu\)
As a test of the practicality of imaginary chemical potential, it is interesting to explore a simple theory that has the sign problem at non-zero chemical potential. The natural candidate is the Hubbard model in 2 dimensions [18,20],

\[
\mathcal{H} = -K \sum_{\langle i,j \rangle, \sigma} a_{i\sigma}^\dagger a_{j\sigma}^\dagger a_{i\sigma} a_{j\sigma} - \frac{U}{2} \sum_i (a_{i\uparrow}^\dagger a_{i\uparrow} - a_{i\downarrow}^\dagger a_{i\downarrow})^2 + \mu \sum_i a_{i\uparrow}^\dagger a_{i\uparrow} - a_{i\downarrow}^\dagger a_{i\downarrow}.
\]  

(9)

By a particle-hole transformation, \(\mu = 0\) gives half-filling. We can replace the four-fermion interaction with an auxiliary field \(A\),

\[
Z(\mu) = \sum_{A(\mathbf{x})} e^{-A^2/2} \det M(\mu) \det M(-\mu).
\]  

(10)

The matrices \(M\), given in [21], are real for real \(\mu\), so the sampling weight is real but not positive, and Monte-Carlo is impossible. For \(\mu\) zero or imaginary, the weight is \(|\det M|^2\), and is positive, so we can calculate ratios of partition functions

\[
\frac{Z(i\nu)}{Z(i\nu_0)} = \sum_{A(\mathbf{x})} e^{-A^2/2} \det M(i\nu) \det M(i\nu_0) /
\]  

and use several values of \(\nu_{\text{update}} = \nu_0\) to eliminate measure-mismatch. In Fig. 5 we show results for \(Z(i\nu)/Z(0)\) using three values of \(\nu_0\). Combining them to obtain a single plot of \(Z(i\nu)/Z(0)\), we see that the three patches agree to within their statistical errors.

Finally, we fit our \(Z(i\nu)\) data to \(\exp(-a\nu^2) \times \text{spline}\), and Fourier transform it to obtain \(Z_N\) (Fig. 4). At this relatively high temperature we have no trouble obtaining \(Z_N\) up to \(N = 5\). It would be interesting to see whether similar results

![Figure 5](image-url)
could be obtained for QCD at temperatures just below the phase transition.

3. Conclusions

In summary, while there are growing indications from Nambu–Jona-Lasinio and other models of exotic phenomena in high-density QCD, it remains very difficult to perform the necessary lattice calculations.

The Glasgow algorithm does not appear to be practical, since even on a $4^4$ lattice it needs more statistics than anyone has been able to gather. Imaginary chemical potential is an interesting alternative, since it is quite possible that the numerical problems of inverse Fourier-transforming $Z_{i\nu}$ to $Z_N$ will be less difficult.

Several other approaches are under development, including perfect actions [22], computer evaluation of the fermionic Grassman integrals [23], and projecting out the $N$-particle sectors using a new dynamical fermion algorithm [24]. Though it is proving hard to find, a successful approach will open up new areas of phenomenology to lattice gauge theorists. Clearly the rewards will be worth the effort.

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