Phase structures of strong coupling lattice QCD with overlap fermions at finite temperature and chemical potential

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(Dated: March 25, 2022)

We perform the first study of lattice QCD with overlap fermions at finite temperature $T$ and chemical potential $\mu$. We start from the Taylor expanded overlap fermion action, and derive in the strong coupling limit the effective free energy by mean field approximation. On the $(\mu, T)$ plane and in the chiral limit, there is a tricritical point, separating the second order chiral phase transition line at small $\mu$ and large $T$, and first order chiral phase transition line at large $\mu$ and small $T$.

PACS numbers: 12.38.Gc, 11.10.Wx, 11.15.Ha, 12.38.Mh

I. INTRODUCTION

To study the nature of matter under extreme conditions in QCD is one of the most challenging issues in particle physics. Several novel phases have been suggested, such as quark-gluon plasma (QCP) and color superconductivity. Precise determination of the QCD phase diagram on the $(\mu, T)$ plane will provide valuable information for these novel phases.

Numerical simulation of lattice gauge theory (LGT) is the most reliable nonperturbative method based on the first principles. This approach has been successfully applied to the findings of the chiral and deconfinement phase transitions at finite $T$ with zero $\mu$. However, LGT experiences serious problems, like species doubling with naive fermions and complex action at finite $\mu$.

The Hamiltonian formulation of LGT at finite density does not have the complex action problem. The complex action problem in Lagrangian formulation forbids numerical simulation at real $\mu$. The recent years have seen enormous efforts on solving the complex action problem, and some very interesting information on the phase diagram for QCD at large $T$ and small $\mu$ has been obtained. QCD at large $\mu$ is of particular importance for neutron star or quark star physics.

There have been several popular approaches to solving the species doubling problem of naive fermions. The staggered fermion approach preserves the remnant of chiral symmetry, but it breaks the flavor symmetry and doesn’t completely solve the species doubling problem. The Wilson fermion approach avoids the doublers and preserve the flavor symmetry, but it explicitly breaks the chiral symmetry; In order to define the chiral limit, one has to do nonperturbative fine-tuning of the bare fermion mass, which seems to be an unnatural method from the physical point of view.

These years have seen increasing interest in the overlap fermion approach, which is claimed to have the properties that chiral symmetry is preserved and species doubling problem may be solved. Chiral symmetry in this approach is not the original form, and therefore one of the conditions of the Nielsen-Ninomiya (NO-GO) theorem is not satisfied. However, the Dirac operator of overlap fermion is nonlocal, and the computational costs for simulating dynamical overlap fermions are typically two orders of magnitude heavier than for the Wilson or KS formulations. It is also very tough to introduce the chemical potential into the action. Before the breakthrough of numerical algorithms for applying overlap fermions to QCD thermodynamics, it is very useful to do an analytical study. At $\mu = 0$ and $T = 0$, this was made possible in Ref. where the generalized overlap fermion approach was introduced by Taylor expansion of the Dirac operator.

In this paper, we study the phase diagram of the strong coupling lattice QCD on the $(\mu, T)$ plane using Taylor expanded overlap fermions. In the chiral limit, we elucidate the phase structure and find lines of first and second order chiral phase transitions, as well as the tricritical point where the two lines join.

The rest of paper is organized as follows. In Sec. we shall give a brief review of the Taylor expanded overlap fermion approach, and rewrite the fermion action in terms of composite operators which transform covariantly under the extended chiral transformation. In Sec. we introduce temperature and chemical potential into the system and derive the effective free energy under mean field approximation. In Sec. we analyze the QCD phase diagram on the $(\mu, T)$ plane in the chiral limit. In Sec. the results are summarized.

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II. FORMULATION OF GO FERMIONS

The action of lattice QCD is given by $S = S_G + S_{F,m}$, where
\[
S_G = -\frac{\beta}{6} \sum_p \text{Tr}(U_p + U_p^\dagger - 2),
\]
\[
S_{F,m} = S_F + m \sum \bar{\psi}(x)\psi(x).
\]
Here $\beta = 6/g^2$, and $U_p$ is the ordered product of link variables $U$ around an elementary plaquette. $S_F$ is the massless fermion action:
\[
aD = a^4 \sum_{x,y} \bar{\psi}(x)D(x,y)\psi(y),
\]
with the overlap Dirac operator $D(x,y)$ defined as
\[
aD = 1 + \frac{1}{\sqrt{X}} \frac{1}{X}
\]
This operator is nonlocal and it is extremely difficult to do analytical calculations. An alternative is proposed in Refs. [15, 20], where the operator $X$ is expressed as
\[
X = A + B \sum_j \gamma_j \Gamma_j^\dagger - C \sum_j \gamma_j \Gamma_j^+,
\]
with
\[
\Gamma_j^-(x,y) = \delta_{x+j,y} U_j(x) - \delta_{x,y+j} U_j^\dagger(y),
\]
\[
\Gamma_j^+(x,y) = \delta_{x+j,y} U_j(x) + \delta_{x,y+j} U_j^\dagger(y),
\]
\[
A = \frac{1}{a}(4\pi - M_0),
\]
\[
B = \frac{rt}{2a},
\]
\[
C = \frac{t}{2a}.
\]
Then, one may expand $D(x,y)$ in powers of the parameter $t$ as
\[
aD_{x,y} = 2\theta(A)\delta_{xy} + \frac{C}{|A|} \sum \gamma_j \Gamma_j^-(x,y) + O(t^2),
\]
where we keep the contributions up to $O(t^2)$. In later discussions, we consider the case of negative $A$, which is expected to have the desired properties of QCD.

In Ref. [15], it was shown that the Ginsparg-Wilson (GW) relation
\[
\gamma_5 D + D \gamma_5 = aD \gamma_5 D
\]
implies an exact symmetry on the lattice, since the Nielsen-Ninomiya theorem is not applicable. It has been verified in Refs. [15, 20] that the $t$-expanded $D(x,y)$ given by Eq. (6) satisfies the GW relation.

The action is invariant under infinitesimal chiral transformation $\psi \to \psi + \delta \psi$ and $\bar{\psi} \to \bar{\psi} + \delta \bar{\psi}$, where
\[
\delta \psi = \varepsilon \gamma_5 (1 - aD)\psi,
\]
\[
\delta \bar{\psi} = \varepsilon \bar{\psi} \gamma_5.
\]
It is easy to show that
\[
\langle \bar{\psi} \gamma_5 \psi \rangle \to \langle \bar{\psi} \gamma_5 \psi \rangle + 2\varepsilon \langle \bar{\psi} (1 - \frac{1}{2}aD) \psi \rangle
\]
under the transformation $\delta \bar{\psi} = \varepsilon \bar{\psi} \gamma_5$. This means that for $m = 0$, the vacuum has an exact chiral symmetry if the vacuum expectation value
\[
\langle \bar{\psi} (1 - \frac{1}{2}aD) \psi \rangle = 0.
\]
Otherwise, the chiral symmetry is spontaneously broken if
\[
\langle \bar{\psi} (1 - \frac{1}{2}aD) \psi \rangle \neq 0.
\]
These properties are very important for studying the chiral phase transition at finite temperature and chemical potential.

Therefore, we could choose the quantity $\langle \bar{\psi} (1 - aD/2) \psi \rangle$ as the chiral order parameter, which will reduce to the conventional one in the continuum limit $a \to 0$. It is more convenient to use the fermion fields $q$ and $\bar{q}$. They are related to $\psi$ and $\bar{\psi}$ by
\[
\bar{q} = \psi, \quad q = \left(1 - \frac{1}{2}aD\right) \psi.
\]
The extended chiral transformation is defined by
\[
\delta q = \varepsilon \gamma_5 q, \quad \delta \bar{q} = \varepsilon \bar{q} \gamma_5.
\]
The chiral order parameter is then given by
\[
\langle \bar{q} q \rangle = \langle \bar{\psi} \left(1 - \frac{1}{2}aD\right) \psi \rangle.
\]
For convenience, we set the lattice spacing $a = 1$. Substituting Eqs. (3), (12), and (14) into Eq. (15), we could rewrite the fermion action in terms of the new fermion fields $\bar{q}$ and $q$:
\[
S_{F,m} = \left(1 + \frac{m}{2}\right) \sum_{x,y} \bar{q}(x)D(x,y)q(y) + m \sum_x \bar{q}(x)q(x) + O(t^2).
\]

III. EFFECTIVE FREE ENERGY OF GO FERMION

In the strong coupling limit, the gluonic action $S_G$ vanishes, and $S \to S_{F,m}$. We introduce the chemical potential $\mu$ into the action Eq. (15) by replacing the link variables in the temporal direction [22] with $U_4(x) \to e^\mu U_4(x)$, and $U_4^\dagger(x) \to e^{-\mu} U_4^\dagger(x)$:
\[
S_{F,m} = \left(1 + \frac{m}{2}\right) \frac{C}{|A|} \sum_x \sum_{i=1}^d \bar{q}(x)\gamma_i U_j(x)q(x + \hat{i})
\]

...
by mean field approximation \[6\]

Here \(d = 3\) is the spatial dimensions.

We use a notation \(x = (\vec{x}, \tau)\) in which \(\vec{x}\) and \(\tau\) represents the spatial and temporal coordinate respectively. The temperature is given by \(T = N_\tau^{-1}\) with \(N_\tau\) the number of temporal lattice sites. We also use a representation of \(\gamma\) matrices described in Ref. [23].

The partition function of the system is

\[
Z = \int D[U_j]D[U_4]D[q]D[\bar{q}] \exp(-S_{F,m}). \tag{17}
\]

To derive the effective free energy \(F_{eff} = -\ln Z/\sum_\tau\) we first integrate over spatial gauge link variables \(U_\vec{x}\), using the \(SU(N_c)\) group integration formulas and Taylor expansion:

\[
\int D[U_j] \exp \left( - \left(1 + \frac{m}{2}\right) \frac{C}{|A|} \sum_x \sum_{j=1}^d \gamma_j \bar{q}(x)q(x) + \gamma_j \bar{q}(x)q(x) \right)
\]

\[
\approx 1 \left(1 + \frac{m}{2}\right)^2 \frac{C}{|A|} \sum_x \sum_{j=1}^d \gamma_j \bar{q}(x)q(x) + \gamma_j \bar{q}(x)q(x), \tag{18}
\]

which should be a good approximation for \(N_f/N_c < 3\).

Next, we linearize the four-fermion term in Eq. (18) by mean field approximation

\[
\sum_x \sum_{j=1}^d \gamma_j \bar{q}(x)q(x) + \gamma_j \bar{q}(x)q(x)
\]

\[
\sim \sum_x \sum_{j=1}^d \bar{q}(x) \gamma_j q(x) + \gamma_j \bar{q}(x)q(x), \tag{19}
\]

where \(\bar{v}\) stands for the chiral condensate \(\langle \bar{q}q \rangle\). Substituting Eqs. (18) and (19) into Eq. (17) the partition function becomes

\[
Z = \int D[U_4]D[q]D[\bar{q}] \exp \left( - S_{F,m}^{eff}(U_4, q, \bar{q}; \bar{v}) \right) \tag{20}
\]

with

\[
S_{F,m}^{eff}(U_4, q, \bar{q}; \bar{v}) = \left(1 + \frac{m}{2}\right) \frac{C}{|A|} \sum_x \left[e^\mu \bar{q}(x)\gamma_4 U_4(x)q(x + \hat{4}) - e^{-\mu} \bar{q}(x + \hat{4})\gamma_4 U_4(x)q(x)\right] + m \sum_x \bar{q}(x)q(x). \tag{21}
\]

The hopping terms between \(\bar{q}\) and \(q\) exist only in the temporal direction.

To compute the remaining integrations, we make a Fourier transformation of the fermion fields

\[
q(\vec{x}, \tau) = \frac{1}{\sqrt{N_\tau}} \sum_{n=1}^{N_\tau} \exp(i k_n \tau) \tilde{q}(\vec{x}, n), \tag{22}
\]

\[
\bar{q}(\vec{x}, \tau) = \frac{1}{\sqrt{N_\tau}} \sum_{n=1}^{N_\tau} \exp(-i k_n \tau) \tilde{q}(\vec{x}, n), \tag{23}
\]

I.e., \(U_4(\vec{x}, \tau)\) is diagonal and independent of \(\tau\).

Substituting Eqs. (22) and (23) into Eq. (20) and integrating out the Grassmann variables [23], we have

\[
\int D[\bar{q}] D[q] \exp \left( - \frac{N_f}{N_\tau} \sum_x N_c \bar{q}(x) \Delta q(x) \right) = (\det \Delta)^{N_f/N_c}, \tag{24}
\]

where the determinant is

\[
\det \Delta = \prod_{\vec{x}} \prod_{\alpha=1}^{N_c} \prod_{n=1}^{N_\tau} \left(2 \left(1 + \frac{m}{2}\right) \frac{d}{N_c} \frac{C}{|A|} \bar{v} - m \right)^2 \times \frac{4C^2}{A^2} \left(1 + \frac{m}{2}\right)^2 \left(\sin \bar{k}_n\right)^2 \right)^{1/2}
\]

\[
= \prod_{\vec{x}} \prod_{\alpha=1}^{N_c} \left[ \frac{2C}{|A|} (1 + m/2) \right]^{N_\tau} \times \left(2 \cosh[N_\tau E] \right) + 2 \cos[N_\tau (\theta_a(\vec{x}) - i \mu)], \tag{25}
\]

with

\[
E = \arcsinh \left[ \frac{2(1 + m/2) \left(\frac{C}{|A|}\right)^2 \bar{v} - m}{2\bar{C} (1 + m/2)} \right],
\]

\[
\bar{k}_n = k_n + \theta_a(\vec{x}) - i \mu. \tag{26}
\]

We then perform the integration over \(U_4\) and obtain

\[
\int D[U_4] (\det \Delta)^{N_f/N_c} \]

As a result, the partition function (17) becomes
\[
Z = \exp \left( -\sum_x (1 + m/2)^2 \frac{dC^2}{N_c A^2} [N_f(\bar{v'})^2] \right) \\
\times \prod_x \left[ \frac{2C}{A} \left( 1 + m/2 \right) \right]^{4N_f} \\
\times \left( 2 \cosh(N_c \mu N_c) + \frac{\sinh((N_c + 1)EN_c)}{\sinh(EN_c)} \right)^{N_f/N_c}. \tag{27}
\]

Consequently, we obtain the effective free energy
\[
F_{eff} = -\ln Z/\left( \sum_x \right) \\
= \left( 1 + \frac{m^2}{2} \right)^2 \frac{dC^2}{N_c A^2} [N_f(\bar{v'})^2] \\
- N_f T \times \ln \left( 2 \cosh \left( \frac{N_c \mu}{T} \right) + \frac{\sinh \left( \frac{(N_c + 1)E}{T} \right)}{\sinh \left( \frac{E}{T} \right)} \right) \\
- 4N_f \ln \left( \frac{2C}{A} \left( 1 + \frac{m}{2} \right) \right). \tag{29}
\]

This formula is simple enough to make an analytical study of the vacuum, helpful in understanding the phase structure of strong coupling lattice QCD.

IV. PHASE STRUCTURE IN THE CHIRAL LIMIT

A. Chiral symmetry spontaneously breaking at \( \mu = T = 0 \)

In case of \( T = 0 \), the effective free energy (24) reduces to a simpler form:
\[
\lim_{T \to 0} F_{eff} = \frac{dN_f}{N_c} (\bar{v'})^2 - N_c N_f \max(\mu, E), \tag{30}
\]
with
\[
E = \text{arcsinh} \left( \frac{d}{N_c} \bar{v'} \right), \tag{31}
\]
and
\[
\bar{v'} = \left| \frac{C}{A} \bar{v} \right|. \tag{32}
\]

At \( \mu = 0 \), the effective free energy becomes
\[
F_{eff}[T = 0, \mu = 0] = \frac{dN_f}{N_c} (\bar{v'})^2 - N_c N_f E. \tag{33}
\]

The rescaled chiral condensate \( \bar{v'} \) is determined by the conditions of minimizing the effective free energy
\[
\frac{\partial F_{eff}}{\partial \bar{v'}} = 0, \quad \frac{\partial^2 F_{eff}}{\partial (\bar{v'})^2} > 0,
\]
from which we get
\[
\bar{v'} = \left( \frac{\sqrt{17} - 1}{2} \right)^{1/2} = O(\bar{v'}) \neq 0, \tag{35}
\]
with the spatial dimension and number of colors taken to be \( d = 3 \) and \( N_c = 3 \) respectively. So the chiral condensate defined in Eq. (14) is
\[
\bar{v} = \langle \bar{q}q \rangle = \langle \bar{v} \left( 1 - \frac{d}{2} D \psi \right) \rangle = O(\bar{v'}) = O(A/C) \neq 0. \tag{36}
\]

Therefore in the strong coupling limit, spontaneous symmetry breaking of the extended chiral symmetry occurs at zero temperature and zero chemical potential. This qualitatively agrees with that obtained from the external source method [19].

B. Chiral symmetry restoration at \( \mu \neq 0 \) and \( T = 0 \)

For small \( \mu \), the effective free energy is the same as Eq. (33), i.e.
\[
F_{eff} = N_f \bar{v'}^2 - 3N_f E. \tag{37}
\]

According to Eq. (37), the effective free energy reaches its global minimum \( F_{min} = -1.971N_f \) at \( \bar{v'} = 1.25 \).

For large enough \( \mu \), the effective free energy (38) reaches its minimum
\[
F_{min} = -3N_f \mu \tag{38}
\]
when \( \bar{v'} = 0 \), i.e., the system is in the chiral symmetric phase.

Therefore, when \( \mu \) increases from zero, the global minimum changes from \(-1.971N_f \) to \(-3N_f \mu \) at the critical chemical potential \( \mu_c \), determined by \(-1.971N_f = -3N_f \mu_c \). Therefore \( \mu_c = 0.657 \), at which the order parameter \( \bar{v'} \) changes discontinuously, as shown in Fig. 1. This is a clear indication of first order chiral phase transition.

C. Chiral symmetry restoration at \( \mu = 0 \) and \( T \neq 0 \)

In the small \( \bar{v'} \) region, the effective free energy takes the form
\[
F_{eff}(\mu, T, \bar{v'}) = C_0(\mu, T) + C_1(\mu, T)\bar{v'}^2 + C_2(\mu, T)\bar{v'}^4 + O(\bar{v'^6}), \tag{39}
\]

where
where

\[ C_0(\mu, T) = -N_f T \ln \left( \frac{2 \cosh(3\mu/T) + 4}{A} \right), \]

\[ C_1(\mu, T) = N_f \left( 1 - \frac{20}{5T + 2T \cosh(3\mu/T)} \right), \]

\[ C_2(\mu, T) = \frac{4N_f}{3T + 2 \cosh(3\mu/T)} \times \left( 5 + \frac{65 - 34 \cosh(3\mu/T)}{T^2(5 + 2 \cosh(3\mu/T))} \right). \]

According to the Landau’s theory, a second order phase transition occurs when the coefficient of $\bar{v}^2$ becomes zero. In the case $\mu = 0$ and $T \neq 0$, there is a critical value for $T = T_c$ at which $C_1(0, T_c) = 0$. In this case, $\bar{v}$ vanishes continuously, implying a second order phase transition at the critical temperature $T_c$, as shown in Fig. 2 when $C_1$ and $C_2$ vanish simultaneously. These results indicate a second order chiral phase transition for $T \geq T_{tri}$ and a first order one for $T < T_{tri}$, as shown in Fig. 3. The existence of the tricritical point is consistent with the recent result from the Hamiltonian approach with Wilson fermion.

D. Phase diagram on the $(\mu, T)$ plane

Finally we study the phase structure on the $(\mu, T)$ plane, based on above discussions. According to Eq. (41), the coefficient of $\bar{v}^2$ vanishes when

\[ \mu_c(T) = \frac{T_c}{3} \arccosh \left( \frac{20 - 5T_c}{2T_c} \right), \]

which corresponds to the second order chiral phase transition line. When the coefficient of $\bar{v}^4$ becomes negative, first order chiral phase transition occurs at some positive value of $C_1$.

Consequently, we have a tricritical point

\[ T_{tri} = 1.241, \quad \mu_{tri} = 0.745. \]

V. DISCUSSION AND OUTLOOK

In the preceding sections, we have made the first attempt to investigate the phase diagram of Lagrangian lattice QCD with overlap fermions at finite temperature $T$ and chemical potential $\mu$. In the strong coupling limit, we discovered a tricritical point on the $(\mu, T)$ plane, separating the second order chiral phase transition line at small $\mu$ and large $T$, and first order chiral phase transition line at large $\mu$ and small $T$. 
There are still some open questions. (1) The strong coupling is far from the continuum limit. (2) As in Refs. 19, 20, we considered only limited terms in Eq. (19). One may have to include infinitive terms in order to completely suppress the doublers. Analytical calculations will be extremely difficult, even at $\mu = T = 0$. Further study of QCD with overlap fermions at finite temperature and chemical potential, ether analytical or numerical, will be very interesting.

**Acknowledgments**

We would like to thank K. Nagao for useful discussions. This work is supported by the Key Project of National Science Foundation (10235040), Key Project of National Ministry of Education (105135), Project of the Chinese Academy of Sciences (KJCX2-SW-N10) and Guangdong Natural Science Foundation (05101821).

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