Phase structure of lattice QCD with Wilson and Neuberger quarks at finite temperature and density

Xiang-Qian Luo†
Department of Physics, Zhongshan University, Guangzhou 510275, China
E-mail: stslxq@zsu.edu.cn

He-Sheng Chen
Department of Physics, Zhongshan University, Guangzhou 510275, China
Department of Physics, Yangzhou University, Yangzhou 225009, China

Xiao-Lu Yu
Department of Physics, Zhongshan University, Guangzhou 510275, China

We review our results for lattice QCD at finite temperature and density from analytical and numerical calculations with Wilson fermions and overlap fermions.

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†Speaker.
1. Introduction

To study the nature of matter in QCD at high temperature $T$ or large quark chemical potential $\mu$ is one of the most challenging issues in particle physics. Several novel phases have been proposed, such as quark-gluon plasma and color superconductivity. Precise determination of the QCD phase diagram on the $(\mu, T)$ plane will provide valuable information for experimental search.

In the continuum, the grand canonical partition function of QCD at finite $T$ and $\mu$ is

$$Z = \text{Tr} \exp \left( -\frac{H - \mu N}{T} \right),$$

where $N$ is particle number operator $N = \int d^3 x \, \psi^\dagger(x) \psi(x)$.

Monte Carlo (MC) simulation of lattice gauge theory (LGT) is the most popular nonperturbative method based on the first principles. This approach has been successfully applied to QCD 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 $\mu$ does not have the complex action problem\cite{1,2,3,4}. The complex action problem in Lagrangian formulation forbids numerical simulation at real $\mu$. The recent years have seen enormous efforts\cite{5,6,7,8} on solving the complex action problem.

There have been several popular approaches to solving the species doubling problem of naive fermions. The staggered (KS) 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.

The overlap fermion approach\cite{9,10} is claimed to have the properties that chiral symmetry is preserved and species doubling problem may be solved. However, the Dirac operator 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.

In this paper, we summarize our study on above issues using Hamiltonian LGT with Wilson fermions, and Lagrangian MC simulations with four flavors of Wilson fermions. We also present some new results from strong coupling analysis of Lagrangian LGT with overlap fermions.

2. Hamiltonian lattice QCD with Wilson fermions

We begin with the QCD Hamiltonian with Wilson fermions $H = H_g + H_f$ at $\mu = 0$ on 1 dimensional continuum time and $d = 3$ dimensional spatial discretized lattice, where

$$H_g = \frac{g^2}{2a} \sum_x \sum_{j=1}^{d} \sum_{\alpha=1}^{8} E_j^\alpha(x) E_j^\alpha(x) - \frac{1}{ag^2} \sum_p \text{Tr} (U_p + U_p^+) - 2,$$

$$H_f = \frac{1}{2a} \sum_x \sum_{j=1}^{d} \left[ \bar{\psi}(x) (\gamma_j - r) U_j(x) \psi(x + \hat{j}) - \bar{\psi}(x) (\gamma_j + r) U_j^+(x - \hat{j}) \psi(x - \hat{j}) \right]$$
\begin{equation}
+ \left( m + \frac{rd}{a} \right) \sum_x \bar{\psi}(x) \psi(x). \tag{2.1}
\end{equation}

According to Eq. (2.1), the role of the Hamiltonian at finite \( \mu \) is played by \( H_\mu = H - \mu N \).

Denoting \( N_f, N_c, V \) the number of flavors, colors, and spatial lattice sites, and \( |\Omega\rangle \) the vacuum state when \( \langle \Omega | H_\mu | \Omega \rangle \) is minimized. For free massless Wilson fermions at \( T = 0 \), we obtained[4] the energy \( \langle \Omega | H | \Omega \rangle = 2N_cN_f \sum_p |p| | \Theta(\mu - |p|) - 1 \rangle \), and the subtracted energy density in the infinite volume limit \( V \rightarrow \infty \) and continuum limit \( a \rightarrow 0 \)

\[
\varepsilon_{sub} = \frac{\langle \Omega | H | \Omega \rangle - \langle \Omega | H_\mu | \Omega \rangle |_{\mu = 0}}{N_cN_fV} = \frac{2}{(2\pi)^3} \int |p| \Theta(\mu - |p|) d^3\vec{p} = \frac{8\pi}{(2\pi)^3} \int_0^\mu p^3 d\mu = \frac{\mu^4}{4\pi^2},
\]

which agrees with the continuum theory. Therefore in the lattice Hamiltonian formulation, the chemical potential could be introduced in a natural way as in the continuum.

For infinitely strongly interacting Wilson fermions, integrating out the gauge fields leads to four fermion interactions[3]. Extreme conditions (large \( T \) or \( \mu \)) induce chiral phase transitions. For \( N_f/N_c < 1 \) with \( N_c = 3 \), we obtained an equation for the critical line where the chiral condensate and the dynamical mass of quark vanish continuously[4]

\[
\mu_\epsilon' = (1 + r^2) \sqrt{1 - \frac{2T_c'}{1 + 3r^2}} + T_c' \ln \frac{1 + \sqrt{1 - \frac{2T_c'}{1 + 3r^2}}}{1 - \sqrt{1 - \frac{2T_c'}{1 + 3r^2}}}. \tag{2.3}
\]

Here we have rescaled the chemical potential and temperature as \( \mu' = \mu/(3K/a) \) and \( T' = T/(3K/a) \), with \( K \) being the effective coupling of four fermion interactions. Below some \( T'_3 \), there is a first order chiral phase transition line[4]

\[
\mu_\epsilon' = 1 + 2r^2, \tag{2.4}
\]

where the chiral condensate and the dynamical mass of quark vanish discontinuously. The point when two lines described by Eq. (2.3) and Eq. (2.4) join at lower \( T' \) is the tricritical point, as shown by the filled circle in Fig. 1.

3. Lagrangian lattice QCD with Wilson fermions

The lattice action at \( \mu = 0 \) proposed by Wilson[11] is \( S = S_g + S_f \), where

\[
S_g = -\frac{\beta}{6} \sum_p \text{Tr}(U_p + U_p^\dagger - 2),
\]

\[
S_f = \sum_{x,y} \bar{\psi}(x) M_{x,y} \psi(y),
\]

\[
M_{x,y} = \delta_{x,y} - \kappa \sum_{j=1}^4 \left[ (r - y_j) U_j(x) \delta_{x,y-j} + (r + y_j) U_j^\dagger(x-j) \delta_{x,y+j} \right], \tag{3.1}
\]

with \( \beta = 6/g^2 \) and \( \kappa = 1/(2ma + 8r) \). The lattice Hamiltonian \( H \) in Eq. (2.1) could also be derived from the Wilson action by Legendre transformation.
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Figure 1: Phase diagram from Hamiltonian lattice QCD with massless Wilson fermions at strong coupling. The solid and dotted lines stand respectively for the first and second order transitions. The circle is the tricritical point.

However, naive introduction of the chemical potential would lead to divergent $\varepsilon_{sub}$ in the continuum limit. In Ref. [12], the chemical potential is introduced by replacing the link variables in the temporal direction in fermion action in Eq. (3.1) with $U_4(x) \rightarrow e^{a \mu} U_4(x)$ and $U_4^\dagger(x) \rightarrow e^{-a \mu} U_4^\dagger(x)$. The fermionic action is reduced to the continuum one when $a \rightarrow 0$.

Nevertheless, the effective fermionic action in the partition function becomes complex, and forbids MC simulation with importance sampling. Several revised methods, e.g., improved reweighting [5] and imaginary chemical potential methods [6, 7], were proposed to simulate QCD with KS fermions at finite $\mu$.

Lattice QCD at imaginary chemical potential $i\mu_I$ does not suffer the complex action problem. In Ref. [8], we applied this method to the MC study of the phase structure of $N_f = 4$ Wilson fermions. We measured the expectation of the Polyakov loop, chiral condensate and their susceptibilities for various $(\mu_I, T)$ at some $\kappa$. From the position of the peak in the susceptibilities, we determine the transition point. Replacing $\mu_I$ by $-i\mu$, we directly continue the transition line on the $(\mu_I, T)$ plane to the real $(\mu, T)$ plane.

Figure 2 is the expected phase diagram of lattice QCD with Wilson fermions in the $(\mu, T, \kappa)$ parameter space. There is a surface $\kappa = \kappa_{chiral}$ where the pion becomes massless. Above this surface, there is no phase transition, as confirmed by our numerical simulations for $\kappa = 0.25$. Interesting physics is below this surface. Of course, the order of transition depends on the value of $\kappa$. For $r = 1$, we find $\kappa_1 \in (0.001, 0.15)$, $\kappa_2 \in (0.15, 0.165)$ and $\kappa_{chiral} \in (0.17, 0.25)$.

4. Lagrangian lattice QCD with overlap fermions

The overlap fermionic action $S_f$ has the form [10]

$$S_f = m \sum_x \bar{\psi}(x) \psi(x) + \sum_{x,y} \bar{\psi}(x) D(x,y) \psi(y),$$

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\[ D = 1 + X \frac{1}{\sqrt{X^4 X}}, \quad (4.1) \]

where \( a \) is set to be 1 for convenience. The operator \( D \) is nonlocal and it is extremely difficult to do analytical calculations. In Ref. [15], we used the Taylor expansion trick [13, 14] to derive an overlap action at finite \( \mu \)

\[ S_f = \left( 1 + \frac{m}{2} \right) \frac{C}{|A|} \left( \sum_x \sum_{j=1}^d \left[ \bar{q}(x) \gamma_j U_j(x) q(x+\hat{j}) - \bar{q}(x+\hat{j}) \gamma_j U_j^\dagger(x) q(x) \right] + \sum_x \left[ e^{\mu x} \bar{q}(x) \gamma_4 U_4(x) q(x+\hat{4}) - e^{-\mu x} \bar{q}(x+\hat{4}) \gamma_4 U_4^\dagger(x) q(x) \right] + m \sum_x \bar{q}(x) q(x) \right), \quad (4.2) \]

where \( A = 4r - M_0 \), and \( C = t/2 \), with \( t \) an expansion parameter. The fermion fields \( q \) and \( \bar{q} \) are related to \( \psi \) and \( \bar{\psi} \) by [14]

\[ \bar{q} = \bar{\psi}, \quad q = \left( 1 - \frac{1}{2} D \right) \psi. \quad (4.3) \]

The chiral order parameter is then given by

\[ \langle \bar{q} q \rangle = \langle \bar{\psi} \left( 1 - \frac{1}{2} D \right) \psi \rangle. \quad (4.4) \]

In Ref. [15], we studied the phase structure of LGT with overlap fermions on the \((\mu, T)\) plane at the strong coupling. The phase diagram is shown in Fig. 3. We find that the phase structure is very similar to the Wilson fermion case.

5. Discussions

LGT with imaginary chemical potential could be used for simulating QCD at small \( \mu \). The overlap fermion approach is a promising one for investigating chiral properties of the phase transition, and the Hamiltonian lattice formulation is a more natural way to introduce chemical potential; However, a lot of efforts have to be made before realistic MC simulations could be carried out.
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Figure 3: Phase diagram of lattice QCD with massless overlap fermions at strong coupling on the $(\mu, T)$ plane. The dotted and solid lines stand respectively for the second and first order transitions. The circle is the tricritical point.

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