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Wilson fermions with imaginary chemical potential

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We study the phase structure of the $N_f = 2$ flavors QCD with imaginary chemical potential with the use of the clover-improved Wilson quark action and renormalization-group improved gauge action. We calculate the Polyakov loop on $8^3 \times 4$ lattice for $(\beta, \kappa) = (1.8, 0.1411), (1.9, 0.1388), (1.95, 0.1377)$ with $\mu_I = 0.2618$. We find that the phase of the Polyakov loop shows a two-state signal indicating the first order phase transition. This transition occurs in the vicinity of $\beta = 1.9$, which corresponds to the temperature $T/T_{pc} = 1.08$.
We also present a reduction formula for the quark determinant of the Wilson fermion. We discuss the feature of the matrix reduction formula.

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1. Introduction

It is of prime interest to understand QCD at finite temperature and density. The lattice QCD with a non-zero baryon density suffers from a sign problem, where the determinant of the quark matrix becomes complex and Monte Carlo simulations become unavailable. Because of this, it is still challenge to understand the QCD at finite density. Several approaches have been investigated to overcome or circumvent the sign problem: multi-parameter reweighting, canonical approaches, imaginary chemical potentials, and so on.

If the chemical potential is pure imaginary $\mu = \mu_R + i\mu_I(\mu_R = 0)$, the quark determinant becomes real due to the identity $\Delta(\mu_I)^\dagger = \gamma_5\Delta(\mu_I)\gamma_5$. Thus, there is no sign problem in this case, and the standard Monte Carlo algorithm can be applied to. The imaginary chemical potential was investigated with the use of the staggered (KS) fermion by De Forcrand and Philipsen [1] and D'Elia and Lombardo [2, 3]. Wu, Luo and Chen considered the imaginary chemical potential using the standard Wilson quark action [4].

The study of the phase structure in (β, μ_I)-plane provides us with an understanding of the phase structure in (β, μ_R)-plane through analytic continuation. In the study of the imaginary chemical potential, it is important to consider the Roberge-Weiss periodicity [5]. In the presence of the quark, the $Z(3)$ symmetry is explicitly broken. However, if the chemical potential is pure imaginary, the $Z(3)$ symmetry is maintained via a translation of μ_I as

$$Z\left(T, \frac{\mu_I}{T}\right) = Z\left(T, \frac{\mu_I}{T} + \frac{2\pi}{N_c}k\right), \tag{1.1}$$

where k is an integer. Roberge and Weiss showed the existence of a phase transition at high temperature, where the phase of the Polyakov loop is an order parameter, while this phase transition does not occur at low temperature. A critical line corresponding to this phase transition is $\frac{\mu_I}{T} = \frac{\pi}{N_c}$ with a critical endpoint T_E, see Fig 1.

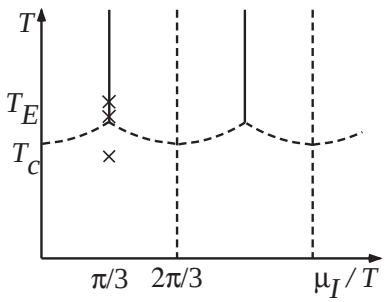

Figure 1: A schematic figure of the phase structure in $(T, \mu_I/T)$ plane. Vertical solid lines show the critical lines of the Roberge-Weiss phase transition. Vertical dashed lines shows the Roberge-Weiss periodicity. The crossed symbols corresponds to points where the present simulations are performed.

In this study, we present two results. First, we report a preliminary results on the study of the phase structure of the $N_f = 2$ flavors QCD with an imaginary chemical potential by using the clover-improved Wilson quark action and renormalization-group improved gauge action on $8^3 \times 4$

lattice for $(\beta,\kappa) = (1.8, 0.1411)$, $(1.9, 0.1388)$, and $(1.95, 0.1377)$ with the imaginary chemical potential $\mu_I = 0.2618$. Second, we present a reduction formula for the quark determinant of the Wilson action, which is an extension of the reduction formula given in Ref [6, 7, 8].

2. Phase Structure with Imaginary Chemical Potential

2.1 Formulation

We employ the renormalization group improved gauge action [9]

$$S_g = \frac{\beta}{6}\left[c_0 \sum(1\times 1 \text{ loop}) + c_1 \sum(1\times 2 \text{ loop})\right], \tag{2.1}$$

with $c_1 = -0.331$ and $c_0 = 1 - 8c_1$ and clover-improved Wilson action, where the quark matrix is written as

$$\begin{aligned}\Delta(x,y) = \delta_{x,x'} &- \kappa \sum_{i=1}^{3}\left[(1-\gamma_i)U_i(x)\delta_{x',x+\hat{i}} + (1+\gamma_i)U_i^\dagger(x')\delta_{x',x-\hat{i}}\right] \\ &- \kappa\left[e^{+\mu}(1-\gamma_4)U_4(x)\delta_{x',x+\hat{4}} + e^{-\mu}(1+\gamma_4)U_4^\dagger(x')\delta_{x',x-\hat{4}}\right] \\ &- \delta_{x,x'} C_{SW}\kappa \sum_{\mu\le\nu}\sigma_{\mu\nu}F_{\mu\nu}.\end{aligned} \tag{2.2}$$

For the coefficient of the clover term C_{SW}, we use a result obtained in the one-loop perturbation theory [10], $C_{SW} = (1-0.8412\beta^{-1})^{-3/4}$. We calculate the Polyakov loop $\langle L\rangle = |L|\exp(i\phi)$, where the phase ϕ is an order parameter of the Roberge-Weiss phase transition [5].

2.2 Results

We perform simulations on $8^3\times 4$ lattice by using the standard hybrid Monte Carlo algorithm. In the present study, we carry out the simulations for three set of parameters $(\beta,\kappa) = (1.8, 0.1411)$, $(1.9, 0.1388)$, and $(1.95, 0.1377)$. All for these three cases, we use a fixed value of the imaginary chemical potential $\mu_I = 0.2618$, which is on the line of the Roberge-Weiss phase transition $\mu_I/T = \pi/N_c$. These parameters correspond to lines of the constant physics with $m_{PS}/m_V = 0.8$ in the absence of the chemical potential [11]. We set a step size of the molecular dynamics to be $\delta\tau = 0.02$ and the number of the molecular dynamics to be 50, which gives the length of a molecular dynamics trajectory to be one. We generate 10, 000 trajectories and measure the Polyakov loop for each trajectory.

Figures 2 show the history of the Monte Carlo simulations for the absolute value and the phase of the Polyakov loop for $\beta = 1.9$. The phase of the Polyakov loop ϕ shows the two-state structure with $\phi = 0$ and $-\pi/3$. This indicates the first order Roberge-Weiss phase transition.

Figure 3 shows the distribution of the phase of the Polyakov loop ϕ, where the first 5,000 steps are removed as thermalization. Following Ref. [11], three sets of the parameters correspond to the temperature $T/T_{pc} = 0.93$ for $(\beta,\kappa) = (1.8, 0.1411)$, $T/T_{pc} = 1.08$ for $(1.9, 0.1388)$ and $T/T_{pc} = 1.20$ for $(1.95, 0.1377)$, where T_{pc} is a pseudocritical temperature. It follows from the figures that at low temperature ($\beta = 1.8$), the system has one vacuum with the value of the order parameter $\phi \sim 0.3$. As temperature becomes higher ($\beta = 1.9$), two-state behavior appears with the

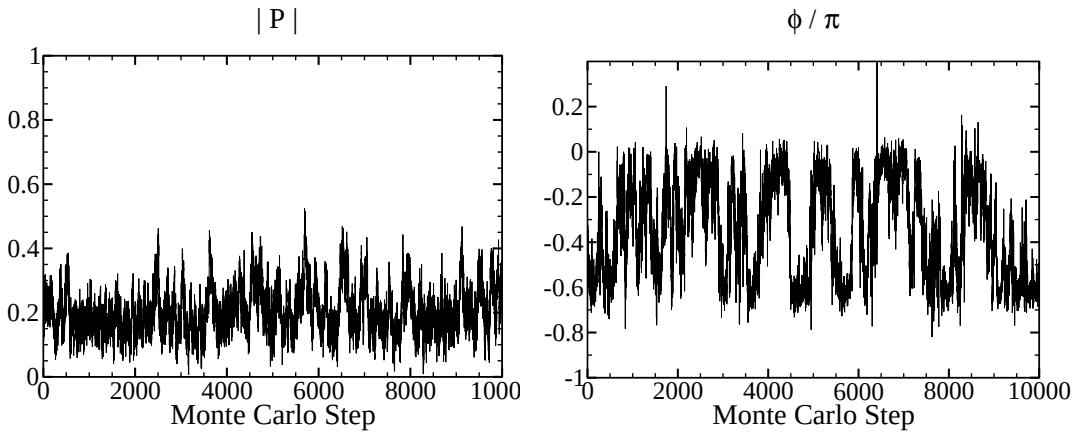

Figure 2: Monte Carlo History of the Polyakov loop for $(\beta,\kappa,\mu_I) = (1.9, 0.1388, 2.618)$. The left panel shows the absolute value $|P|$ and the right panel shows the phase ϕ.

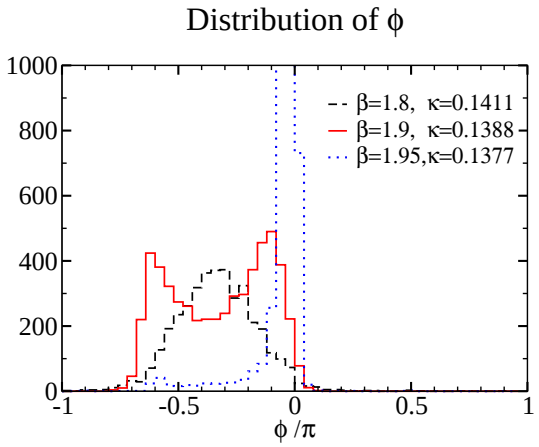

Figure 3: A histogram of the distribution of the phase of the Polyakov loop ϕ. The dashed (black), solid (red) and dotted (blue) lines correspond to $(\beta,\kappa) = (1.9, 0.1411), (1.9, 0.1388)$ and $(1.95, 0.1377)$, respectively. We use the same value of the imaginary chemical potential $\mu_I = 0.2618$ for these three sets of the parameters.

two vacua $\phi = 0$ and $\phi = -\pi/3$, although the peak structure is not sharp due to the small lattice size. As temperature becomes much higher ($\beta = 1.95$), the vacuum shift to $\phi = 0$. We find the onset of the Roberge-Weiss phase transition is in the vicinity of $\beta = 1.9$ for which $T/T_{pc} = 1.08$. This is almost consistent with the previous result obtained by the standard Wilson quark action [4]. On the other hand, the phenomenological approaches [12, 13, 14, 15] reported larger values $T_E = 200 \sim 210$ MeV. This dicrepancy is probably caused by the fact that we employed large quark mass $m_{ps}/m_V \sim 0.8$.

3. Gibbs formula for Wilson fermions

In this section, we derive a formula which is indispensable if we use Wilson fermions for

the multiparameter reweighting by Fodor and Katz (i.e., using no Taylor expansion) [8], and also for the canonical expression. Danzer, Gattringer and Liptak studied a decomposition of the quark determinant for Wilson action[16, 17]. Here we derive an alternative expression.

We can write Wilson fermion matrix as

$$\Delta = B - z^{-1}\kappa(r-\gamma_4)V - z\kappa(r+\gamma_4)V^\dagger, \tag{3.1}$$

where

$$\begin{aligned} B(x,x') \equiv\ & \delta_{x,x'} - \kappa\sum_{i=1}^{3}\left\{(r-\gamma_i)U_i(x)\delta_{x',x+\hat{i}} + (r+\gamma_i)U_i^\dagger(x')\delta_{x',x-\hat{i}}\right\} \\ & + (Clover), \end{aligned} \tag{3.2}$$

and

$$V(x,x') \equiv U_4(x)\delta_{x',x+\hat{4}}. \tag{3.3}$$

We introduce z as $z \equiv e^{-\mu}$. Now we rewrite Δ:

$$\begin{aligned} \det\Delta &= \det(B - z^{-1}\kappa(r-\gamma_4)V - z\kappa(r+\gamma_4)V^\dagger), \\ &= z^{-N}\begin{vmatrix} -BV - z(-\kappa(r+\gamma_4)) & I \\ \kappa(r-\gamma_4)V^2 & -z \end{vmatrix} / \det V\ , \\ &= z^{-N}\left|\begin{pmatrix} -BV & I \\ \kappa(r-\gamma_4)V^2 & 0 \end{pmatrix} - z\begin{pmatrix} -\kappa(r+\gamma_4) & 0 \\ 0 & I \end{pmatrix}\right|. \end{aligned} \tag{3.4}$$

Here N is a rank of the block matrices, such as B and V, $N \equiv N_c \times 4 \times N_x N_y N_z N_t$. By exchanging the columns and raws, this matrix now reads

$$\det\Delta = z^{-N}\det(T - zS). \tag{3.5}$$

Here we describe the matrices T and S as block matrices in time-plane,

$$T = \left(\begin{array}{c|c|ccc|c} 0 & t_1 & 0 & \cdots & & 0 \\ \hline 0 & 0 & t_2 & \cdots & & 0 \\ \hline 0 & 0 & 0 & \cdots & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & \cdots & t_{N_t-2} & 0 \\ \hline 0 & 0 & & \cdots & 0 & t_{N_t-1} \\ \hline t_{N_t} & 0 & & \cdots & 0 & 0 \end{array}\right), \quad S = \left(\begin{array}{c|c|ccc|c} s & 0 & 0 & \cdots & & 0 \\ \hline 0 & s & 0 & \cdots & & 0 \\ \hline 0 & 0 & 0 & \cdots & & \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \hline 0 & 0 & & \cdots & s & 0 \\ \hline 0 & 0 & & \cdots & 0 & s \end{array}\right), \tag{3.6}$$

where

$$t_i = \begin{pmatrix} -B_i V_{i,i+1} & 1 \\ \kappa(r-\gamma_4)V_{i-1,i}V_{i,i+1} & 0 \end{pmatrix}, \quad s = \begin{pmatrix} -\kappa(r+\gamma_4) & 0 \\ 0 & I \end{pmatrix}.$$

Each t_i and s is $(4N_cN_xN_yN_z) \times (4N_cN_xN_yN_z)$ matrix.

Even though the matrix S does not have an inverse, the formula (3.5) can be evaluated by the generalized eigen value problem,

$$T\vec{X} = zS\vec{X}. \tag{3.7}$$

Namely the generalized Schur decomposition[18] tells us that there exist unitary Q and Z such that $Q^\dagger SZ$ and $Q^\dagger TZ$ are upper triangular. We write their diagonal elements, α_i and β_i, respectively. Then

$$\det(T - zS) = \det(QZ^\dagger)\prod_i(\alpha_i - z\beta_i). \tag{3.8}$$

This is a Gibbs formula for Wilson fermions. However, we evaluated α_i and β_i using LAPACK routine, and there is an accuracy problem. Then we go further to obtain a satisfactory formula.

Let us rewrite the determinant of $T - zS$ as

$$\det(T - zS) = \begin{vmatrix} t_{N_t} & 0 & \cdots & 0 & -zs \\ -zs & t_1 & 0 & \cdots & 0 \\ 0 & -zs & t_2 & \cdots & 0 \\ 0 & 0 & -zs & \cdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & & & \cdots\ t_{N_t-2} & 0 \\ 0 & 0 & \cdots & -zs & t_{N_t-1} \end{vmatrix}. \tag{3.9}$$

We multiply matrices Q_1 and Q_2 from the right

$$Q_1 = \begin{pmatrix} I & 0 & \cdots & t_{N_t}^{-1}zs \\ 0 & I & 0\ \cdots & 0 \\ 0 & 0 & I\ \cdots & 0 \\ \cdots & \cdots & \cdots\ \cdots & \cdots \\ & & \cdots & 0 \\ 0 & 0 & \cdots & I \end{pmatrix},\ Q_2 = \begin{pmatrix} I & 0 & \cdots & t_1^{-1}zst_{N_t}^{-1}zs \\ 0 & I & 0\ \cdots & 0 \\ 0 & 0 & I\ \cdots & 0 \\ \cdots & \cdots & \cdots\ \cdots & \cdots \\ & & \cdots & 0 \\ 0 & 0 & \cdots & I \end{pmatrix}. \tag{3.10}$$

Here $\det Q_1 = \det Q_2 = 1$. Then, we obtain

$$\begin{aligned} \det(T - zS) &= \det(T - zS)Q_1Q_2, \\ &= |t_{N_t}| \\ &\times \begin{vmatrix} t_1 & 0 & \cdots & 0 \\ -zs & t_2 & \cdots & -zst_1^{-1}zst_{N_t}^{-1}zs \\ 0 & -zs & \cdots & \\ \cdots & \cdots & \cdots\ \cdots & \cdots \\ & & \cdots\ t_{N_t-2} & 0 \\ 0 & & \cdots\ -zs & t_{N_t-1} \end{vmatrix}, \\ &= |t_{N_t}| \times |t_1| \times \\ &\begin{vmatrix} t_2 & \cdots & -zst_1^{-1}zst_{N_t}^{-1}zs \\ -zs & \cdots & \\ & \cdots\ \cdots & \cdots \\ & \cdots\ t_{N_t-2} & 0 \\ 0 & \cdots\ -zs & t_{N_t-1} \end{vmatrix}. \end{aligned} \tag{3.11}$$

We go further recursively.

$$\begin{aligned}\det(T-zS) &= \det(T-zS)Q_1Q_2\cdots Q_{N_t-2},\\ &= |t_{N_t}|\times|t_1|\times\cdots|t_{N_t-3}|\\ &\times \begin{vmatrix} t_{N_t-2} & -zst_{N_t-3}^{-1}zs\cdots t_1^{-1}zst_{N_t}^{-1}zs\\ -zs & t_{N_t-1}\end{vmatrix}.\end{aligned} \tag{3.12}$$

Since

$$\begin{pmatrix} t_{N_t-2} & -zst_{N_t-3}^{-1}zs\cdots t_1^{-1}zst_{N_t}^{-1}zs\\ -zs & t_{N_t-1}\end{pmatrix} = \begin{pmatrix} t_{N_t-2} & 0\\ 0 & I\end{pmatrix}\times\begin{pmatrix} I & -t_{N_t-2}^{-1}zst_{N_t-3}^{-1}zs\cdots t_1^{-1}zst_{N_t}^{-1}zs\\ -zs & t_{N_t-1}\end{pmatrix}, \tag{3.13}$$

we obtain

$$\begin{aligned}\det(T-zS) &= |t_{N_t}|\times|t_1|\times\cdots|t_{N_t-2}|\\ &\times \quad |t_{N_t-1}-zst_{N_t-2}^{-1}zst_{N_t-3}^{-1}zs\cdots t_1zst_{N_t}^{-1}zs|,\\ &= |t_{N_t}|\times|t_1|\times\cdots|t_{N_t-2}|\times|t_{N_t-1}|\\ &\times \quad |I-t_{N_t-1}^{-1}zst_{N_t-2}^{-1}zst_{N_t-3}^{-1}zs\cdots t_1zst_{N_t}^{-1}zs|,\\ &= |P|\times|I-z^{N_t}t_{N_t-1}^{-1}st_{N_t-2}^{-1}st_{N_t-3}^{-1}s\cdots t_1st_{N_t}^{-1}s|,\end{aligned} \tag{3.14}$$

where $P=t_1t_2\cdots t_{N_t}$.

Therefore, the ratio of the fermion determinant with $z=e^{-\mu}$ to that with $z=1$, i.e., $\mu=0$ is

$$\frac{\det\Delta(\mu)}{\det\Delta(\mu=0)} = z^{-N}\frac{\det\left(I-z^{N_t}Q\right)}{\det\left(I-Q\right)}. \tag{3.15}$$

Here Q is a matrix of $L\times L$ with $L\equiv 2\times 4\times N_cN_xN_yN_z$ and is given as

$$Q\equiv t_{N_t-1}^{-1}st_{N_t-2}^{-1}st_{N_t-3}^{-1}s\cdots t_1st_{N_t}^{-1}s. \tag{3.16}$$

If we can diagonalize $Q\to\mathrm{diag}\{q_1,q_2,\cdots,q_L\}$, then

$$\frac{\det\Delta(\mu)}{\det\Delta(\mu=0)} = z^{-N}\frac{\prod_{l=1}^{L}(1-z^{N_t}q_l)}{\prod_{l=1}^{L}(1-q_l)}. \tag{3.17}$$

Although it contains inverse matrix calculations, t^{-1}, the matrix Q does not depend on N_t.

4. Summary

We have investigated the phase structure of the QCD with the imaginary chemical potentials. We employed $N_f=2$ flavors QCD with the renormalization-group improved gauge action and the clover-improved Wilson quark action. We performed simulations on $8^3\times 4$ lattice for $(\beta,\kappa)=(1.8,0.1411),(1.9,0.1388),(1.95,0.1377)$ with $\mu_I=0.2618$. We found that the phase of

the Polyakov loop showed the two-state signals at $(\beta,\kappa) = (1.9, 0.1388)$, which indicates the first order phase transition. This phase transition occurs in the vicinity of $\beta = 1.9$, which corresponds to $T/T_{pc} = 1.08$. In order to understand the phase structure of the QCD, such as the pseudocritical line $\beta_c(\mu)$ and the endpoint of the Roberge-Weiss phase transition, the simulation for other values of (β,κ,μ_I) is in progress.

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