QCD phase transition at real chemical potential with canonical approach

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Abstract

We study the finite density phase transition in the lattice QCD at real chemical potential. We adopt canonical approach and the canonical partition function is constructed for $N_f = 2$ QCD. After derivation of the canonical partition function we calculate observables like the pressure, the quark number density, its second cumulant and the chiral condensate as a function of the real chemical potential. We covered a wide range of temperature region starting from the confining low to the deconfining high temperature. We observe signals for the deconfinement and the chiral restoration phase transition at real chemical potential below $T_c$ starting from the confining phase.
I. INTRODUCTION

The grand canonical ensemble is a difficult subject to treat in lattice QCD because of the sign problem. The canonical partition function is related to the grand canonical one through the fugacity expansion and is known to be free from the complex action problem. The history of the canonical approach in finite density lattice QCD may have started with a development of a reduction formula for the Dirac determinant [1], which gives naturally a fugacity expansion of the Dirac determinant. A several studies with the staggered fermion are done along this line [2–5] and have been taken over by the Wilson fermion [6–10]. Since it is understood that the inverse transformation of the fugacity expansion is the Fourier transformation [3] it also becomes a popular method [11–15].

One of the problem of the canonical approach is that the Dirac determinant needs to be evaluated accurately, which is the heaviest part of the computation. One of the solution is to adopt the Taylor expansion [16]. In this paper we perform the fugacity expansion by a method of the hopping parameter expansion in temporal direction: winding number expansion [12, 13]. By using the hopping parameter expansion the Dirac determinant can be evaluated with low cost and we can visit a wide parameter space in $\beta$. The canonical partition function is evaluated for $N_f = 2$ QCD both in the deconfinement and the confinement temperature regions. After derivation of the canonical partition function we study the chemical potential dependence of observables like the pressure, the quark number density and the chiral condensate. We observe signals for the confinement-deconfinement and chiral restoration phase transition at real chemical potential below the critical temperature $T_c$. A preliminary result has been reported in Ref. [17].

This paper is organized as follows. In Sec. 2 we briefly review the canonical approach. Our formulation of the fugacity expansion in terms of the hopping parameter expansion is discussed in Sec. 3. After mentioning our numerical setup in Sec. 4 our main results are given in Sec. 5 for the canonical and grand canonical partition functions. Sec. 6 is devoted for the chiral condensate in grand canonical ensemble. A conclusion is given in Sec. 7.
II. CANONICAL PARTITION FUNCTION

It is a well known fact that the grand canonical ensemble and the canonical one are equivalent each other. This is shown by a simple equation to relate the grand canonical partition function $Z_G(\mu, T, V)$ and the canonical $Z_C(n, T, V)$

$$Z_G(\mu, T, V) = \sum_{n=-\infty}^{\infty} Z_C(n, T, V) \xi^n, \quad \xi = e^{\mu/T}. \quad (1)$$

This is a so called fugacity expansion formula. The inverse of this expansion is given by using the Cauchy’s integral theorem

$$Z_C(n, T, V) = \oint d\xi \frac{2\pi i}{2\pi i} \xi^{-n-1} Z_G(\xi, T, V), \quad (2)$$

where we assume that the partition function $Z_G(\xi, T, V)$ has singularities only at $\xi = 0, \infty$ corresponding to trivial ones $\mu/T = \pm \infty$ and adopt an appropriate contour around the origin. Here we notice that a phase transition point $\xi_c$ is not a singularity of the partition function but it is rather a zero of $Z_G(\xi, T, V)$ (Lee-Yang zeros [18, 19]) and does not affect the Cauchy’s integral.

Now it is free to change the contour to a unit circle $\xi = e^{i\theta}$ and the contour integral turns out to be a Fourier transformation

$$Z_C(n, T, V) = \int_0^{2\pi} d\theta e^{-in\theta} Z_G(e^{i\theta}, T, V). \quad (3)$$

A standard Monte Carlo simulation is possible for the lattice QCD since the chemical potential is set to pure imaginary $\mu/T = i\theta$ and the Boltzmann weight is real positive for two flavors.

However a difficulty of the sign problem is preserved unfortunately since there remains a frequent cancellation in plus and minus sign in a numerical Fourier transformation especially for large particle numbers. In order to get the canonical partition function accurately for large quark number $n$ we need a very fine sampling of $Z_G(e^{i\theta}, T, V)$ in $\theta$. This requires a heavy computational cost because we need to evaluate the Dirac operator determinant for the QCD grand partition function. In this paper we shall solve this problem by a direct expansion of the Dirac determinant in terms of the fugacity.
III. WINDING NUMBER EXPANSION

We consider the lattice $N_f = 2$ QCD grand partition function given in the path integral form

$$Z_G(\xi, T, V) = \int DU \left( \text{Det} D_W(\xi; U) \right)^2 e^{-S_G(U)},$$

where we adopt the improved Wilson Dirac operator

$$D_W = 1 - \kappa Q,$$

$$Q = \sum_{i=1}^{3} \left( Q_i^+ + Q_i^- \right) + e^{\mu a} Q_4^+ + e^{-\mu a} Q_4^- + T,$$

$$\left( Q_{\mu}^+ \right)_{nm} = (1 - \gamma_{\mu}) U_{\mu}(n) \delta_{m,n+\hat{\mu}}, \quad \left( Q_{\mu}^- \right)_{nm} = (1 + \gamma_{\mu}) U_{\mu}^\dagger(m) \delta_{m,n-\hat{\mu}},$$

$$\left( T \right)_{nm} = c_{SW} \frac{1}{2} \sum_{\mu,\nu} \sigma_{\mu\nu} F_{\mu\nu}(n) \delta_{nm}$$

Both the chemical potential $e^{\pm \mu a}$ and the hopping parameter $\kappa$ appear in front of the temporal hopping term simultaneously. The fugacity expansion of the determinant shall be given by using the hopping parameter expansion.

Instead of the determinant we consider the hopping parameter expansion of

$$\text{TrLog} D_W = \text{TrLog} (I - \kappa Q) = -\sum_{n=1}^{\infty} \frac{\kappa^n}{n} \text{Tr}(Q^n).$$

A non-trivial chemical potential dependence appears when the quark hoppings make a loop in the temporal direction. If one of the term has a $n$ times winding loop in positive temporal direction, the chemical potential dependence is $e^{\mu a N_t}$ where $N_t$ is a temporal lattice length and this is nothing but $e^{n\mu/T} = \xi^n$. Counting the winding number in temporal direction for each term in equation (9), we get the winding number expansion of the TrLog

$$\text{TrLog} D_W(\mu) = \sum_{n=-\infty}^{\infty} w_n \xi^n.$$

Regrouping the summation, we have a fugacity expansion of the determinant

$$\text{Det} D_W(\xi; U) = \exp \left( \sum_{n=-\infty}^{\infty} w_n \xi^n \right) = \sum_{n=-\infty}^{\infty} z_n(U) \xi^n.$$

In this approach, the fugacity dependence of the determinant or the partition function is given analytically. A numerical Fourier transformation can be executed safely at any
### Table I: \( \beta \) and \( \kappa \) for the numerical simulation. \( m_\pi/m_\rho \) is also given.

| \( \beta \) | \( \kappa \) | \( m_\pi/m_\rho \) |
|---|---|---|
| 0.9 | 0.137 | 0.8978(55) |
| 1.1 | 0.133 | 0.9038(56) |
| 1.3 | 0.138 | 0.809(12) |
| 1.5 | 0.136 | 0.756(13) |
| 1.7 | 0.129 | 0.770(13) |
| 1.9 | 0.125 | 0.714(15) |
| 2.1 | 0.122 | 0.836(47) |

In this paper, extraction of the coefficient \( z_n(U) \) from the second term in equation (11) is done by using the multi-precision numerical Fourier transformation. The winding number expansion is done for gauge configurations generated at \( \mu_0 = 0 \) or purely imaginary value. This procedure corresponds to the standard reweighting method

\[
Z_G(\xi,T,V) = \int DU \left( \frac{\text{Det} D_W(\mu)}{\text{Det} D_W(\mu_0)} \right)^2 \text{Det} D_W(\mu_0)^2 e^{-S_G}. \tag{12}
\]

**IV. NUMERICAL SETUP**

We adopt the Iwasaki gauge action and the improved Wilson fermion action with the clover term. The number of flavors is set to \( N_f = 2 \) with degenerate masses. The APE stout smeared gauge link [20] is used for those in the fermion action including the clover term. The number of smearing is four and the parameter is set to \( \rho = 0.1 \). The clover coefficient is fixed to \( c_{SW} = 1.1 \) [21]. We adopt \( 8^3 \times 4 \) lattice. A wide range of \( \beta \) is covered from high temperature \( \beta = 2.1 \) to low temperature 0.9. It seems to be that both the confining and deconfining region are well covered, which is inferred from a behavior of real part of the Polyakov loop in the left panel of Fig. 1. The temperature corresponding to \( \beta = 1.7 \) seems to be very near to the critical \( T_c \) as is shown the right panel of Fig. 1 using a fluctuation of phase of the Polyakov loop. The hopping parameter is selected in order that the hopping parameter expansion works well, for which \( m_\pi/m_\rho \) turns out to be 0.7 - 0.9 as is given in table I. Maximal order of the hopping parameter expansion is set to 480 so that max winding number in temporal direction is 120. Number of independent configuration is 100 - 600.
FIG. 1: Real part of the Polyakov loop as a function of $\beta$ (left). Both the confining and deconfining regions are well covered. Right panel is a fluctuation of phase of the Polyakov loop. $\beta = 1.7$ seems to be very near to the critical coupling.

FIG. 2: The canonical partition function $\log |Z_C(n_B)/Z_C(0)|/(VT^3)$ as a function of the baryon number $n_B$. From the top $\beta = 2.1$ (orange), 1.9 (red), 1.7 (magenta), 1.5 (green), 1.3 (dark green), 1.1 (blue), 0.9 (black).

V. CANONICAL AND GRAND CANONICAL PARTITION FUNCTION

The first numerical result we get is the canonical partition function $Z_C(n, T, V)$. We plot $\log |Z_C(n_B, T, V)/Z_C(0, T, V)|/(VT^3)$ as a function of the baryon number $n_B$ in Fig. 2. The partition function decays very rapidly with $n_B$ and its behavior changes drastically between $\beta = 1.9$ (red) and 1.5 (green), which may correspond to a phase transition.

The plot range is fixed by using the d’Alembert’s convergence condition

$$\lim_{n_B \to \infty} \left| \frac{Z_C(n_B + 1)}{Z_C(n_B)} \right| < 1,$$

(13)
FIG. 3: Log plot of $|Z_C(n_B + 1)/Z_C(n_B)|$ as a function of the baryon number. The color and $\beta$ correspondence is the same as in Fig. 2 for left panel. Right panel is that at $\beta = 1.1$ and $2.1$ for example.

which gives the convergence radius for the fugacity $\xi$. The data at $\beta = 1.1$ and $2.1$ are plotted in right panel of Fig. 3 for example. We cut our data at $n_{\text{max}}$ where a monotonic decrease stops indicated by vertical orange and blue lines in the figure. The horizontal lines show maximal values of the fugacity expected to be within the convergence radius. By taking log, the line gives our applicable limit for the baryon chemical potential $\mu_B/T$. For example we can discuss physics safely at $-10 < \mu_B/T < 10$ for $\beta = 1.1$ and $-4 < \mu_B/T < 4$ for $\beta = 2.1$ with our method. We notice that $n_{\text{max}}$ is improved only by one even if we increase the maximal winding number twice as $120 \rightarrow 240$. This may be due to a fact that the convergence radius of the Taylor expansion is unity.

The second physical quantity is the grand partition function. By taking summation for $-n_{\text{max}} \leq n_B \leq n_{\text{max}}$ in equation (1), we get the grand partition function for the real chemical potential. Here we notice that the canonical partition function $Z_C(n, T, V)$ is a real positive quantity if a Hermitian transfer matrix exists for the lattice QCD. We observed that the absolute value of the partition function is very stable against the statistical fluctuation and we consider it is suitable for extracting physical information. Instead of equation (1) we adopt

$$Z_G(\mu, T, V) = \sum_{n=-n_{\text{max}}}^{n_{\text{max}}} |Z_C(n, T, V)| \xi^n$$

(14)

\footnote{For negative baryon number we adopt $|Z_C(n_B - 1)/Z_C(n_B)|$.}
FIG. 4: The grand partition function \( \log \left| \frac{Z_G(\mu, T, V)}{Z_G(0, T, V)} \right| \) as a function of the quark chemical potential \( \mu/T \). The color and \( \beta \) correspondence is the same as in Fig. 2. The pressure at \( \beta = 0.9 \) and 1.1 are plotted in the upper left panel, where two data are completely overlapped. The upper right panel is that at \( \beta = 1.3 \) and 1.5. Lower panel is that for \( \beta = 1.7, 1.9, 2.1 \).

for a definition of the grand partition function \(^2\), from which we get the pressure in the grand canonical ensemble

\[
\frac{1}{T^4} (P(\mu/T) - P(0)) = \frac{1}{VT^3} \log \left| \frac{Z_G(\mu, T, V)}{Z_G(0, T, V)} \right|. \tag{15}
\]

We plot the pressure normalized at \( \mu = 0 \) in Fig. 4 as a function of the quark chemical potential. We observe that the pressure is almost consistent with zero for small chemical potential at low temperature below \( T_c \) as is shown in the upper panels of Fig. 4.

The third physical application is the \( k \)-th momentum of the quark number operator

\[
\langle \hat{N}^k \rangle = \frac{1}{Z_G(\mu, T, V)} \sum_{n=-n_{\text{max}}}^{n_{\text{max}}} n^k Z_C(n, T, V) \xi^n. \tag{16}
\]

\(^2\) Notice this is not a phase quenching of the Dirac determinant.
FIG. 5: Quark number density $\langle \hat{N} \rangle / (VT^3)$ as a function of the quark chemical potential. The color and $\beta$ correspondence is the same as in Fig. 2. The upper panels plot results for $\beta = 0.9 - 1.5$ below $T_c$. The lower panel is results for $\beta = 1.7 - 2.1$ above $T_c$.

In Fig. 5, the quark number density $\langle \hat{N} \rangle / (VT^3)$ is plotted as a function of the real quark chemical potential $\mu/T$. We observe a Silver blaze like phenomenon at low temperature below $T_c$ as is shown in the upper panels. The quark number density is consistent with zero within a statistical error until $\mu/T \sim 1$ is reached. Above $\mu/T \sim 1$ the quark number density takes off and becomes non-zero, which indicates deconfinement phase transition.

The second cumulant of the quark number density may be a good indicator of this phase transition. The results at low temperature side below $T_c$ are plotted in the upper panels of Fig. 6. Those above $T_c$ are given in the lower panel. We observe peaks around $\mu/T \sim 1$ below $T_c$ for every $\beta$ in the upper panels. We also observe secondary peaks for $\beta = 1.3$ (dark-green) and 1.5 (green) at larger $\mu/T \geq 2$ in the upper right panel. Only a single peak is observed at high temperature in the lower panel. These peaks have a distinctive behavior against the quark number cut-off $n_{\text{max}}$. The first peaks below $T_c$ are stable even if we vary $n_{\text{max}}$ by 20%. On the other hand, the second peaks at $\beta = 1.3, 1.5$ and the first peaks above
FIG. 6: The second cumulant of the quark number $\langle \hat{N}_q^2 \rangle_c / (VT^3)$ as a function of the quark chemical potential. The upper panels plot results for $\beta = 0.9 - 1.5$ below $T_c$. The lower panel is results for $\beta = 1.7 - 2.1$ above $T_c$.

$T_c$ change their height and position with $n_{\text{max}}$. It would be conjectured that the first peaks in the low temperature side are the physical indication of the confinement-deconfinement phase transition. The secondary peaks below $T_c$ and the peaks in the high temperature side would be artifacts due to the cut-off in quark number in the fugacity expansion.

The thermodynamical quantity

$$\frac{\mu}{T} = -\frac{\partial \ln Z_C(n, T, V)}{\partial n} = -\frac{1}{V} \frac{\partial \ln Z_C(\rho V, T, V)}{\partial \rho} \quad (17)$$

as a function of the baryon number density is one of the post popular quantity in the canonical approach \[5, 8, 13, 16\]. We notice the quantity plotted in Fig. 3 can be interpreted as an expression of the derivative in terms of the differential

$$\frac{\mu}{T} = -\frac{1}{3} \left( \ln Z_C(n_B + 1, T, V) - \ln Z_C(n_B, T, V) \right). \quad (18)$$

The results are plotted in Fig. 7. Although the error is rather large there seems to appear a typical S-shape like behavior at small baryon density $\rho_B / T < 0.5$ for the low temperature
FIG. 7: The quark chemical potential \( \mu/T \) given in terms of the thermodynamical relation as a function of the baryon number density. The upper panels plot results for \( \beta = 0.9 - 1.5 \) below \( T_c \). The lower panel is results for \( \beta = 1.7 - 2.1 \) above \( T_c \).

side given in the upper panels, which may indicate an existence of the first order phase transition.

VI. HADRONIC OBSERVABLES

In our procedure, the fugacity expansion is based on the hopping parameter expansion. It may be possible to expand any hadronic operators in terms of the fugacity. We consider a fugacity expansion of a numerator of some operator vacuum expectation value (VEV)

\[
\langle O \rangle_G(\xi, T, V) = \frac{O_G(\xi, T, V)}{Z_G(\xi, T, V)},
\]

\[
O_G(\xi, T, V) = \int DU \langle O \rangle_{\text{quark}}(\xi) \text{Det}D_W(\xi; U)e^{-S_G(U)} = \sum_{n=-\infty}^{\infty} O_C(n, T, V)\xi^n,
\]

where \( \langle O \rangle_{\text{quark}} \) is a Wick contraction of a hadronic operator \( O \) in quark fields. For example, we consider the chiral condensate. It is easy to expand its Wick contraction in terms of the
hopping parameter

\[
\langle \bar{\psi} \psi \rangle_{\text{quark}} = -\text{tr} \left( \frac{1}{D_W} \right) = -\text{tr} \left( \frac{1}{1 - \kappa Q} \right) = \sum_{m=0}^{\infty} \kappa^m \text{tr} Q^m = \sum_{n=-\infty}^{\infty} o_n(U) \xi^n. \tag{21}
\]

Counting the winding number in temporal direction, we get the last equality. Multiplying the determinant contribution (11), we apply the same regrouping procedure in Sec. III and get the fugacity expansion (20).

Once we have two coefficients \( Z_C(n,T,V) \) and \( O_C(n,T,V) \), the VEVs of the operator with the canonical and the grand canonical ensemble are available. The canonical ensemble VEV is given by taking the ratio of two coefficient

\[
\langle O \rangle_C(n,T,V) = \frac{O_C(n,T,V)}{Z_C(n,T,V)}. \tag{22}
\]

The result for the chiral condensate \(-\int d^3x \langle \bar{\psi} \psi \rangle_C/(VT^3)\) is given in the left panel of Fig. 8 as a function of the baryon number.

A VEV in the grand canonical ensemble is given by taking fugacity summation with real chemical potential

\[
\langle O \rangle_G(\xi,T,V) = \frac{\sum_{n=-n_{\text{max}}}^{n_{\text{max}}} O_C(n,T,V) \xi^n}{\sum_{n=-n_{\text{max}}}^{n_{\text{max}}} Z_C(n,T,V) \xi^n}. \tag{23}
\]

The chiral condensate \(-\int d^3x \langle \bar{\psi} \psi \rangle_G/(VT^3)\) is given in the right panel of Fig. 8 as a function of the real chemical potential \(\mu/T\). The condensate in the figure is a bare quantity without renormalization. Since we adopted the Wilson fermion, we have an additive correction for \(\langle \bar{\psi} \psi \rangle\), which is not subtracted in this paper. From the figure, the chiral restoration phase transition at finite chemical potential seems to be seen. A relatively large value at around \(\mu/T = 0\) starts to decrease rapidly at chemical potential \(\mu/T \sim 1\) for low temperature. The would-be transition parameter \(\mu_c/T\) becomes larger for lower temperature and smaller for high temperature although we need to notice the quark mass is not the same for each \(\beta\). The position of \(\mu_c/T\) seems to be consistent with that of the first peak for the second cumulant in the upper panels of Fig. 6.

The quark number density is also given in terms of the hadronic observable \(\int d^3x \langle \bar{\psi} \psi \rangle/(VT^3)\), which gives consistent result with that in Sec. 5 up to renormalization factor as is plotted in Fig 9.
FIG. 8: The chiral condensate $-\int d^3x \langle \bar{\psi}\psi \rangle / (VT^3)$ in the canonical ensemble (left panel) as a function of the baryon number. The right panel is that in the grand canonical ensemble as a function of the quark chemical potential $\mu/T$. The color and $\beta$ correspondence is the same as in Fig. 2.

FIG. 9: The quark number density $\int d^3x \langle \psi^\dagger \psi \rangle / (VT^3)$ in the grand canonical ensemble as a function of the quark chemical potential $\mu/T$. The color and $\beta$ correspondence is the same as in Fig. 2.

VII. CONCLUSION

In this paper, we performed the fugacity expansion of the grand partition function by using the hopping parameter expansion. This procedure seems to be valid for baryon numbers around $n_B \sim 30$ for $8^3 \times 4$ lattice and $m_\pi/m_\rho > 0.7$. The method is also applied to the numerator of VEVs of hadronic operators. Taking summation over quark numbers we get a VEV at the real chemical potential. As an example we evaluate the pressure, the quark
number density and its second cumulant and the chiral condensate. These observables show
a phase transition like behavior at high chemical potential for low temperature region, which
may correspond to the confinement-deconfinement or the chiral restoration phase transition.

One of the biggest anxiety in this paper may be an overlap problem due to the reweighting
\[^{(12)}\]. We performed a test of this problem by adopting \(\mu_0/T = 0.5\) for configurations
generation. We find all the results are consistent within the statistical error as we shall
report in the forthcoming paper.

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