Density of States Method at Finite Isospin Density

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Abstract

The density of states method is applied for lattice QCD at a finite isospin density. The advantage of this method is that one can easily obtain results for various values of parameters (quark mass, coupling constant and the number of flavors). We compare results for the chiral condensate and the quark number density with those from the R-algorithm and find that they are in good agreement. By calculating the chiral condensate we obtain information on the phase structure for various quark flavors and isospin chemical potentials. We also show results for the chiral condensate at two different quark masses and at two different isospin densities which are not easily obtainable in the conventional Monte Carlo method.

1 Introduction

The lattice QCD Monte Carlo technique has been a useful tool for clarifying the non-perturbative aspects of QCD at the zero baryon chemical potential ($\mu_B = 0$) for both finite and zero temperatures. At nonzero $\mu_B$, however, due to the sign problem, the standard importance sampling method fails. The Glasgow group\cite{1} attempted to extract information on $\mu_B$ at low temperature by a method based on reweighting but this method does not work at low temperatures due to the overlap problem. Recently it has been realized that at low density and finite temperature the sign problem may not be a serious numerical difficulty and a variety of approaches (multi-reweighting, Taylor expansion, imaginary chemical potential)\cite{2,3,4,5,6} have been applied to study QCD at low density and finite temperature (See\cite{7,8,9,10} for recent reviews). For larger $\mu_B$ we are still lacking an efficient numerical method.

In contrast to the finite $\mu_B$ case, QCD at isospin density has no sign problem and can be simulated by lattice Monte Carlo methods\cite{11}. There is an expectation that at small isospin density the system may resemble that at small baryon density\cite{6,12}. Recent studies have shown that the phase diagram at small isospin density is similar to that at small $\mu_B$\cite{13,14}. On the other hand, a difference between the isospin and baryon density is seen in susceptibilities of number density and derivatives of meson mass\cite{2,15}.

In lattice Monte Carlo simulations, usually importance sampling is used. This approach have been proven to be very efficient by many studies. Another approach one may take is the density of states (DOS) method. The difference between importance sampling and the DOS method is as follows. In importance sampling a simulation is performed at a fixed parameter set. To explore different parameters one must perform independent simulations\footnote{If the parameter region to be explored is narrow, then one may apply the reweighting method\cite{16} which does not need independent simulations.}. On the other hand, in the DOS method one
first determines the DOS of suitable observables and then results are obtained by performing one or a few dimensional integral. To illustrate how the DOS method works, let us consider a gauge model. The partition function for this model is given by

\[ Z = \int [dU] \exp(-\beta S_g[U]), \]

where \( S_g[U] \) is a gauge action and \( \beta \) is a coupling constant. If we define the DOS by

\[ n(E) = \int [dU] \delta(E - S_g[U]), \]

then the partition function is rewritten as

\[ Z = \int dE n(E) \exp(-\beta E). \]

If we consider the average value of the gauge action, it is given by

\[ \langle E \rangle = \int dE n(E) E \exp(-\beta E)/Z. \]

This is a one-dimensional integral of \( E \) and once we obtain \( n(E) \), we can evaluate this easily at any \( \beta \). No extra simulation is needed to calculate it at various \( \beta \), which is considered to be an advantage of this method.

The DOS method has been applied for gauge theories: \( Z(\text{n}), \text{SU}(2) \) and \( \text{SU}(3) \) models\cite{17}. Although the inclusion of dynamical fermions is computationally difficult, in Ref.\cite{18} the DOS method was applied for QED, where the method is called the microcanonical fermionic average method. Recently, Luo\cite{19} extended the idea of the DOS method to QCD and emphasized that once the eigenvalues of the Dirac operator and the DOS of the plaquette energy are determined, one can evaluate the thermodynamic quantities derived from the partition function at any quark mass and flavor.

In this study we apply the DOS method for QCD at isospin density on a 4\( ^4 \) lattice and demonstrate how the DOS method works. Since the isospin system has no sign problem, results from the DOS method can be compared with those from the standard method. In Sec.2 we give general formulas for forming the DOS including dynamical fermions. In Sec.3 we give simulation details. Results are presented in Sec.4. We summarize our results in Sec.5.

## 2 Density of States Method

### 2.1 General Formulas

In lattice QCD Monte Carlo simulations, usually we aim at obtaining the average values of observables:

\[
\langle O \rangle = \frac{1}{Z} \int [dU] O[U] \det \Delta(m_q, \mu)^{N_f/4} \exp(-\beta S_g[U]),
\]

where \( N_f \) is the number of flavors and \( \Delta(m_q, \mu) \) is assumed to be a staggered fermion matrix at quark mass \( m_q \) and at chemical potential \( \mu \):

\[
\Delta(m_q, \mu)_{i,j} = m_q \delta_{i,j} + \frac{1}{2} \sum_{\nu=1,2,3} \eta_{i,\nu}(U_{i,\nu} \delta_{i,j-\nu} - U_{i-\nu,j}^\dagger \delta_{i,j+\nu})
\]

\[
+ \frac{1}{2} \eta_{i,4}(e^{\mu}U_{i,4} \delta_{i,j-4} - e^{-\mu}U_{i-4,j}^\dagger \delta_{i,j+4}).
\]

\( S_g[U] \) is the standard Wilson gauge action,

\[
S_g[U] = \frac{1}{N_c} \sum_p \Re Tr(U_p),
\]

where \( U_p \) is the plaquette and \( N_c = 3 \) for \( \text{SU}(3) \) gauge theory. For Wilson fermions, \( N_f/4 \) in eq.\cite{11} should be replaced with \( N_f \). The standard means of dealing with this multi-dimensional integral is to do the importance sampling, i.e. configurations are generated with a measure \( \sim dU \det \Delta^{N_f/4} e^{-\beta S_g} \).
and $\langle O \rangle$ is given by an average over the configurations as $\langle O \rangle \approx \frac{1}{N} \sum_{i=1}^{N} O[U_i]$, where $N$ is the number of configurations.

The DOS method rewrites the partition function and reduces it to a few dimensional integral. Let us define the DOS with parameters $E_i$ ($i = 1, \ldots, k$) as

$$n(E_1, E_2, \ldots, E_k) = \int [dU] g(U) \Pi_i \delta(E_i - x_i(U)), \quad (4)$$

where $x_i(U)$ is an operator associated with $E_i$ and $g(U)$ is introduced to generalize the DOS further with $g(U) \neq 1$. Using the DOS, we obtain

$$\langle O \rangle = \frac{1}{Z_n} \int [\Pi_i dE_i] n(E_1, E_2, \ldots, E_k) \langle O \det \Delta_{N_f/4} e^{-g(E) / g(U)} \rangle_{E_1, E_2, \ldots, E_k}, \quad (5)$$

where

$$Z_n = \int [\Pi_i dE_i] n(E_1, E_2, \ldots, E_k) \langle \det \Delta_{N_f/4} e^{-g(E) / g(U)} \rangle_{E_1, E_2, \ldots, E_k}. \quad (6)$$

Here, $\langle A \rangle_{E_1, E_2, \ldots, E_k}$ stands for an average of $A$ on configurations generated with the measure $[dU] g(U) \Pi_i \delta(E_i - x_i(U))$, or one can write it as

$$\langle A \rangle_{E_1, E_2, \ldots, E_k} = \frac{1}{n(E_1, E_2, \ldots, E_k)} \int dU g(U) \Pi_i \delta(E_i - x_i(U)) A(U). \quad (7)$$

For $g(U) = 1$, $\langle A \rangle_{E_1, E_2, \ldots, E_k}$ becomes a microcanonical average at fixed $E_1, E_2, \ldots, E_k$.

**2.2 $g(U) = 1$**

Here we give the formulas used in the present study. We consider the case of one parameter and choose $x(U) = S_g[U]$. Although there are many possibilities to choose $x(U)$, this choice with $g(U) = 1$ is the one used in Ref. [19] and is useful for our purpose. Setting $g(U) = 1$, we obtain

$$n(E) = \int [dU] \delta(6VE - S_g[U]), \quad (8)$$

$$\langle O \rangle = \frac{1}{Z_n} \int dE n(E)e^{-6VE}\langle O \det \Delta(\mu)^{N_f/4} \rangle_{E}, \quad (9)$$

and

$$Z_n = \int dE n(E)e^{-6VE}\langle \det \Delta(\mu)^{N_f/4} \rangle_{E}, \quad (10)$$

where $V$ is the number of lattice sites and $E$ is the plaquette energy. These are the basic formulas used in our study. Our task includes three numerical calculations: (i) $n(E)$, (ii) $\langle \det \Delta(\mu)^{N_f/4} \rangle_{E}$ and (iii) $\langle O \det \Delta(\mu)^{N_f/4} \rangle_{E}$. Luo [19] argued that if one stores the eigenvalues of the fermion matrix for all configurations, then one can evaluate $\langle \det \Delta(\mu)^{N_f/4} \rangle_{E}$ for any quark mass and flavor. Let $\lambda_i(\mu)$ be the $i$-th eigenvalue of the massless fermion matrix $\Delta(m_q = 0)$ on a configuration with $E$. Then we obtain

$$\langle \det \Delta(\mu)^{N_f/4} \rangle_{E} = \langle \left( \prod_{i} \lambda_i(\mu) + m_q \right)^{N_f/4} \rangle_{E}. \quad (11)$$

Since (iii) contains $O$, in general it is not calculable for any quark mass and flavor. However the chiral condensate $\langle \bar{\psi} \psi \rangle$ which is obtained as the trace of the inverse fermion matrix can also be given with the eigenvalues. Namely, for $\langle \bar{\psi} \psi \rangle$ we obtain

$$\langle \left( \frac{1}{V} Tr \Delta(\mu)^{-1} \right) \det \Delta(\mu)^{N_f/4} \rangle_{E} = \langle \frac{1}{V} \sum_{i} \frac{1}{\lambda_i(\mu) + m_q} \left( \prod_{i} \lambda_i(\mu) + m_q \right)^{N_f/4} \rangle_{E}. \quad (12)$$

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2.3 \( g(U) \neq 1 \)

Depending on the purpose, one may take \( g(U) \neq 1 \). In Ref.\[20\] the DOS for the complex phase of the fermion determinant was calculated. The DOS was defined as

\[
n(E) = \int [dU] g(U) \delta(E - \theta(U)),
\]

where \( g(U) \) is set to \(| \text{det} \Delta | e^{-\beta S_{\text{det}}(U)} | \), and \( \theta(U) \) is the complex phase of the determinant. Then the expectation value of \( O \) is given by

\[
\langle O \rangle = \frac{\int_0^\pi \beta^{E} n(E) e^{iE} \int_0^\pi \beta^{E} n(E) e^{iE}}{\int_0^\pi \beta^{E} n(E) e^{iE}}.
\]

In Ref.\[21\] the DOS for the number density was used and \( g(U) \) is also set to \(| \text{det} \Delta | e^{-\beta S_{\text{det}}(U)} | \).

In these definitions parameters \( \beta \) and \( m_q \) are absorbed in \( n(E) \) and we cannot vary \( \beta \) and \( m_q \). Therefore, in this study we do not use these definitions with \( g(U) \neq 1 \).

3 Simulations

For the case of \( N_f = 2 \), we have two chemical potentials \( \mu_u \) and \( \mu_d \) associated with the \( u \) and \( d \) quarks respectively. If we introduce the isospin chemical potential \( \mu_I \) as \( \mu_I \equiv \mu_u = -\mu_d \), we obtain

\[
[\text{det} \Delta(\mu_u)\Delta(\mu_d)]^{1/4} = [\text{det} \Delta(\mu_I)\Delta(-\mu_I)]^{1/4} = | \text{det} \Delta(\mu_I) |^{1/2},
\]

which is positive in the Monte Carlo measure. Therefore, for this \( \mu_I \) the sign problem is absent and one can perform Monte Carlo simulations. The natural generalization of the isospin chemical potential to \( N_f \neq 2 \) is that one takes \( \text{det} \Delta(\mu_I)^{N_f/4} \equiv | \text{det} \Delta(\mu_I) |^{N_f/4} \).

We follow the implementation developed in Ref.\[19\]. The DOS \( n(E) \) in eq.\(8\) can be obtained using the quenched data as

\[
- \frac{\ln n(E)}{V} = 6 \int_0^E dE' \beta(E') + \text{const.}
\]

First we make quenched simulations on a \( 4^4 \) lattice and determine the coupling constant \( \beta(E) \) as a function of the plaquette \( E \) (Figure 1). Then we integrate \( \beta(E) \), numerically interpolating the data according to the trapezoidal rule. Figure 2 shows the result of \( - \ln n(E)/V \).

The most time consuming part of our method is the calculations of the microcanonical averages \( \langle \text{det} \Delta(\mu_I)^{N_f/4} \rangle_E \) and \( \langle O \text{ det} \Delta(\mu_I)^{N_f/4} \rangle_E \) as a function of \( E \), which contain the eigenvalue calculations. In order to generate configurations at \( E \) we use the over-relaxation method\[22, 19\]. Starting from a configuration with \( E \), we have made the over-relaxation update and saved 100 configurations at each \( E \). Each configuration is separated by 100 over-relaxation updates. About 30 values of \( E \) are chosen in \( E \in [0.05, 0.95] \). For each configuration we calculate the eigenvalues of the fermion matrix and store them. Using these eigenvalues we can evaluate \( \langle \text{det} \Delta(\mu_I)^{N_f/4} \rangle_E \) as in eq.\(11\) for any quark mass and flavor. Examples of \( \langle \text{det} \Delta(\mu_I)^{N_f/4} \rangle_E \) are shown in Figure 3. Eq.\(12\) is evaluated similarly. These data are interpolated by polynomials when we perform eqs.\(8\)-\(10\).
4 Results

Figures 4 and 5 compare results of $\langle \bar{\psi} \psi \rangle$ between the DOS method and the R-algorithm \[23\]. We see a good agreement between them in a wide range of $\beta$. A small difference is seen in the phase transition region where the $\langle \bar{\psi} \psi \rangle$ changes rapidly. In such a region we probably need careful analysis.

Figure 6 shows $\langle \bar{\psi} \psi \rangle$ for different $N_f$ at $m_q = 0.025$ and $\mu_I = 0.2$(left), and at $m_q = 0.05$ and $\mu_I = 0.25$(right) as functions of $\beta$. One can see that the critical coupling where the phase transition occurs decreases as $N_f$ increases. Figure 7 shows $\langle \bar{\psi} \psi \rangle$ for various $\mu_I$. In the low-temperature phase $\langle \bar{\psi} \psi \rangle$ decreases as $\mu_I$ increases. On the other hand, in the high-temperature phase no visible difference can be seen among $\langle \bar{\psi} \psi \rangle$. Since the DOS method can explore various parameter space easily it is considered to be useful for exploring a wide parameter space and for seeing a rough phase diagram.

In the DOS method we can take various combinations of parameters. Let us consider the case of $N_f = 1 + 1$ with non-degenerate quark masses $m_1$ and $m_2$. In this case we must calculate the following microcanonical averages:

$$\langle | \det \Delta(m_1) |^{N_f/4} | \det \Delta(m_2) |^{N_f/4} \rangle_E,$$  \hspace{1cm} (17)

$$\langle \bar{\psi} \psi(m_{i=1,2}) | \det \Delta(m_1) |^{N_f/4} | \det \Delta(m_2) |^{N_f/4} \rangle_E.$$  \hspace{1cm} (18)
Figure 3: Microcanonical average of $\det \Delta(\mu_I)^{N_f/4}$ at $\mu_I = 0.2$ and $m_q = 0.025$ as a function of $E$.

Since the eigenvalues are stored, it is easy to calculate these microcanonical averages. On the other hand, in the conventional algorithm such as R-algorithm one needs a differently implemented program to simulate $N_f = 1+1$. Such a program can be implemented but may become intricate.

Figure 4: $\langle \bar{\psi}\psi \rangle$ for $N_f = 2$ at $m_q = 0.05$ and at $\mu_I = 0.0$ (left) and 0.2 (right). Circles are from the DOS method. The results from the R-algorithm are shown with squares.

Next we show the results of the number density $n_d$ defined by

\[ n_d = \frac{1}{V} \frac{1}{\partial \ln Z} = \frac{1}{V} Tr \left( \frac{1}{\Delta(\mu)} \frac{\partial \Delta(\mu)}{\partial \mu} \right). \] (21)
Since this cannot be evaluated with the eigenvalues of $\Delta(\mu)$ only, in order to obtain $\langle O \mid \det \Delta(\mu) \rangle^{N_f/4}_E$ for the number density we must calculate the number density on each configuration.

Usually Eq. (21) is evaluated by the noise method. Using noise vectors $R_i$ having the property $\langle R_i^\dagger R_j \rangle = \delta_{ij}$, the trace calculation can be replaced by

$$Tr \frac{1}{\Delta(\mu)} \frac{\partial \Delta(\mu)}{\partial \mu} = \frac{1}{N} \sum_{i=1}^{N} R_i^\dagger \frac{1}{\Delta(\mu)} \frac{\partial \Delta(\mu)}{\partial \mu} R_i,$$

where $N$ is the number of noise vectors. Although this is true for $N \to \infty$, we find that the convergence of the noise method is extremely slow on a $4^4$ lattice. A similar result was reported in Ref. [24]. Figure 10 shows the convergence measured as relative error as a function of the number of $Z_2$ noise vectors [25]. Typically, $O(1000)$ noise vectors are needed to have a reasonable value. In this analysis, instead of using the noise method we calculated the number density exactly by calculating each diagonal element of $\frac{1}{\Delta(\mu)} \frac{\partial \Delta(\mu)}{\partial \mu}$. In general such calculations are computationally costly and should be avoided. However, our lattice size is sufficiently small to perform the exact calculation. Thus, here we have adopted the exact calculation.
Figure 7: $\langle \bar{\psi} \psi \rangle$ for different $\mu_I$. (left) $N_f = 2$ and $m_q = 0.05$. (right) $N_f = 4$ and $m_q = 0.025$.

Figure 8: $\langle \bar{\psi} \psi (m_q) \rangle$ for $N_f = 1 + 1$ at $\mu_I = 0.2$ with different quark masses, $m_q = 0.05$ and 0.025.

Figure 11 shows the number density as a function of $\mu_I$. The results from the R-algorithm are also plotted in the figure. The two results are in good agreement.

5 Summary and outlook

We have given the general formulas of the DOS method including dynamical fermions. The case of "$g(U) = 1$" corresponds to that used by Luo[19]. Based on the implementation by Luo, we have calculated $\langle \bar{\psi} \psi \rangle$ and the number density at finite isospin densities by the DOS method and made a comparison with results from the R-algorithm. The two results were found to be in good agreement. The DOS method can be applied for various combinations of parameters. We have calculated $\langle \bar{\psi} \psi \rangle$ for various values of $N_f$ and $\mu_I$, and also for non-degenerate quark masses and for different isospin chemical potentials. Especially it is emphasized that for non-degenerate quark masses and for different isospin chemical potentials it is not easy to perform Monte Carlo simulations by the conventional algorithm as the R-algorithm but these calculations are easily performed in the DOS method by keeping all eigenvalues of the fermion matrix.

The limitation of the DOS method may appear on a large lattice. The measurement of the DOS method is done in the microcanonical ensemble and $\langle \text{det} \Delta \rangle$ is treated as an observable. Since the
microcanonical and full ensembles are very different, \( \langle \text{det } \Delta \rangle \) is expected to fluctuate largely as the volume of the system increases, which may limit the available lattice to a small one.

In principle, the DOS method can be applied for QCD with a baryon chemical potential. However, there still remains the sign problem. For example, for \( N_f = 4 \) we have \( \langle \text{det } \Delta(\mu_B) \rangle_E = \langle |\text{det } \Delta(\mu_B)|e^{i\theta} \rangle_E \) and if \( e^{i\theta} \) fluctuates significantly, which is expected to occur for larger \( \mu_B \), one cannot obtain meaningful values for the microcanonical average. We attempted to calculate \( \langle |\text{det } \Delta(\mu_B)|e^{i\theta} \rangle_E \) but for \( \mu_B > 0.2 \) we could not obtain statistically meaningful values\(^2\). On the other hand, for \( \mu_B < 0.2 \) the results were stable but there is no visible difference between the results of \( \langle \bar{\psi}\psi \rangle \) at \( \mu_I \) and at \( \mu_B \); for \( \mu_B < 0.2 \) the effect of the complex phase is small and thus we do not see any difference. This is consistent with the results of Refs.\(^{26, 27}\).

In this study for each value of \( \mu \) we calculated the eigenvalues. However, if we use a matrix reduced to two time slices\(^{28, 9}\), we can calculate the determinant at any \( \mu \). The determinant for this case is expressed as

\[
\text{det } \Delta(\mu) = \text{det}(P + e^{N_t\mu}) \times e^{3V\mu},
\]

where \( P \) is a \( \mu \)-independent matrix and \( N_t \) is the number of lattice sites in the time direction. Keeping the eigenvalues of \( P \), we can calculate the determinant at any \( \mu \). In this case, however, the tradeoff is that the determinant is not calculable at any \( m_q \). Thus, if one wishes to obtain the behavior with \( \mu \) at fixed \( m_q \) this reduction method may be useful.

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\(^{2}\)Here \( \mu_B \) is defined as the quark chemical potential.
Figure 10: Relative error of the number density for different $\mu$ at $m_q = 0.025$ as a function of the number of noise vectors. A representative quenched configuration at $\beta = 5.5$ was used. $n_v$ is the number density calculated by the noise method and $n_t$ is the true value of the number density. $Z_2$ noise vectors are used for these calculations. We also used Gaussian noise vectors and obtained similar results.

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Figure 11: Number density as a function of $\mu_I$.

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