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Winding number expansion for the canonical approach to finite density simulations

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The canonical partition function approach was designed to avoid the overlap problem that affects the lattice simulations of nuclear matter at high density. The method employs the projections of the quark determinant on a fix quark number sector. When the quark number is large, the evaluation of the projected determinant becomes numerically unstable. In this paper a different evaluation method based on expanding the determinant in terms of loops winding around the lattice is studied. We show that this method is stable and significantly faster than our original algorithm. This greatly expands the range of quark numbers that we can simulate effectively.

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1. Introduction

To simulate QCD at finite density, the usual approach based on the grand canonical partition function is to split the fermionic determinant into two parts: a real and positive part used to generate an ensemble of configurations, and a complex phase which is folded into the observables. This approach has two major drawbacks: the sign problem and the overlap problem. In order to address the overlap problem, a method which employs the canonical partition function has been proposed [1].

To generate ensembles using this method, the projected determinant for a fixed net quark number (number of quarks minus the number of anti-quarks) needs to be calculated using the Fourier transform of the fermionic determinant [2, 3]. To evaluate it, a discrete version of the Fourier transform was used [2] which was shown to be accurate [3] for quark numbers as large at 15. However, when simulating larger lattices, to achieve the same densities we need to use a proportionally larger number of quarks. As it turns out, the discrete Fourier transform becomes unstable when we use quark numbers larger than 20. To overcome this problem, we have developed a winding number expansion method (WNEM), a method based on the expansion in terms of quark loops. Using this approach, we can evaluate reliably the projected determinant for large quark numbers.

2. Canonical approach

The canonical partition function for lattice QCD is related to the grand-canonical partition function via the fugacity expansion

$$Z(V,T,\mu) = \sum_k Z_c(V,T,k) e^{\mu k/T}, \tag{2.1}$$

where k is the net number of quarks and Z_c is the canonical partition function. Thus, the canonical partition function can be written as a Fourier transform of the grand-canonical partition function

$$Z_c(V,T,k) = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} Z(V,T,\mu)|_{\mu=i\phi T}. \tag{2.2}$$

In this paper, we will consider only the case of two degenerate flavors. If we denote M as the quark matrix for one quark flavor, we have

$$\begin{aligned} Z_c(V,T,k) &= \int \mathscr{D}U e^{-S_G[U]} \det{}_k M^2[U] \\ &= \int \mathscr{D}U e^{-S_G[U]} \det M^2[U] \frac{|\mathrm{Re}\det{}_k M^2[U]|}{\det M^2[U]} \frac{\det{}_k M^2[U]}{|\mathrm{Re}\det{}_k M^2[U]|}, \end{aligned} \tag{2.3}$$

where

$$\det{}_k M^2[U] = \int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} \det M^2[U,\phi] \tag{2.4}$$

is the projected determinant with a fixed net quark number k.

3. Discrete Fourier transform instability

The simplest way to compute the Fourier transform, Eq. (2.4), is to replace the continuous transform with its discrete version,

$$\widetilde{\det}_k M^2[U] = \frac{1}{N}\sum_{j=0}^{N-1} e^{-ik\phi_j} \det M^2[U,\phi_j] \qquad \phi_j = \frac{2\pi j}{N}. \tag{3.1}$$

Unfortunately, the Fourier transform becomes unstable when the quark number k is large as we can see from Table 1. This is a well known problem; it is a consequence of the fact that the higher Fourier components are the result of very delicate cancellations in a a sum of alternating terms.

k	3	6	9	12	15
N=51	2212.21	247.601	-22.8783	-4.53755	-0.233997
N=102	2212.21	247.601	-22.8783	-4.53755	-0.233997
N=204	2212.21	247.601	-22.8783	-4.53755	-0.233997
k	18	21	24	27	30
N=51	-0.00545724	-0.0000602919	6.70879E-7	6.70879E-7	-0.0000602919
N=102	-0.005458	-0.0000631063	-8.98294E-7	1.56917E-6	2.81435E-6
N=204	-0.005458	-0.0000634881	-1.66312E-6	-2.83726E-7	6.42123E-6

Table 1: The projected determinant for a particular configuration with different choices of N. For k larger than 20 the results differ for different choices of N, signaling a numerical instability.

For our studies using $6^3 \times 4$ lattices, to investigate the phase diagram at non-zero baryon densities, we need quark numbers of the order $k \sim 30$ which corresponds to 10 baryons. To evaluate the projection accurately we need a better method.

4. Winding number expansion method

The basic idea of the new method is to use the Fourier transform of $\log\det M(U,\phi)$ instead of the Fourier components of $\det M(U,\phi)$. Using an approximation based on the first few components of $\log\det M(U,\phi)$ we can then analytically compute the projected determinant. The success of the method can be traced to the fact that the Fourier components of $\log\det M(U,\phi)$ are exponentially smaller with increasing order in the expansion [1]. This is why we can approximate the exponent very accurately with few terms which, in turn, allows us to evaluate the Fourier components of the determinant precisely.

To see how this works we look at the hopping expansion of the $\log\det M(U,\phi)$. We start by writing the determinant in terms of its log

$$\det M(U,\phi) = \exp(\mathrm{Tr}\log M(U,\phi)). \tag{4.1}$$

It is well known that $\mathrm{Tr}\log M$ corresponds to a sum of connected quark loops. We separate all these loops in classes in terms of the net number of times they wrap around the lattice in the "time"

[1] This property is also noted in a similar context in [5].

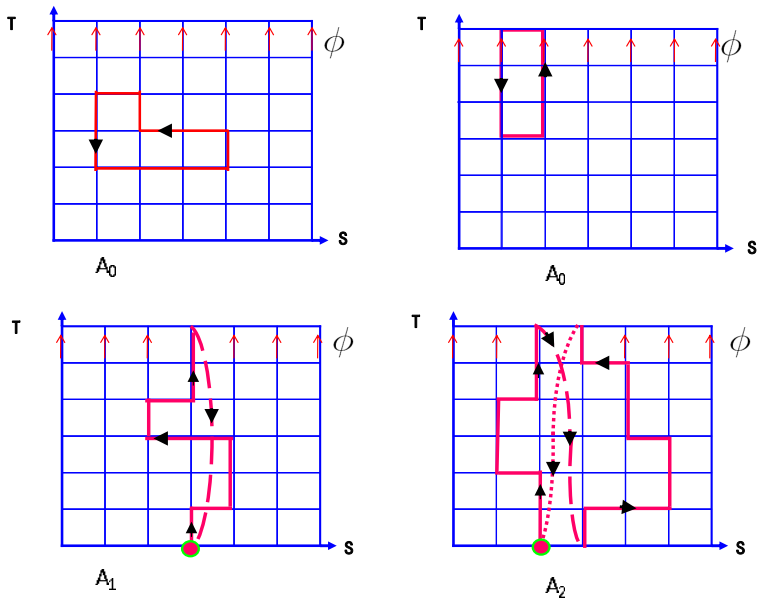

Figure 1: Schematic of winding number expansion on lattice.

direction (see Fig. 1). We have then:

$$\begin{aligned} \mathrm{Tr}\log M(U,\phi) &= \sum_{\text{loops}} L(U,\phi) \\ &= A_0(U) + [\sum_n e^{in\phi} W_n(U) + e^{-in\phi} W_n^\dagger(U)], \end{aligned} \tag{4.2}$$

where n is winding number of quark loops and W_n is the weight from the contribution of all the quark loops which have fixed winding number n in time direction. Eq. (4.2) can be re-written as

$$\begin{aligned} \mathrm{Tr}\log M(U,\phi) &= A_0(U) + [\sum_n e^{in\phi} W_n(U) + e^{-in\phi} W_n^\dagger(U)] \\ &= A_0(U) + \sum_n A_n \cos(n\phi + \delta_n), \end{aligned} \tag{4.3}$$

where $A_n \equiv 2|W_n|$ and $\delta_n \equiv \arg W_n$ are independent of ϕ. Using Eq. (4.1) and Eq. (4.3) we get

$$\det M(U,\phi) = e^{A_0 + A_1\cos(\phi+\delta_1) + A_2\cos(2\phi+\delta_2) + \ldots..}. \tag{4.4}$$

To first order in the winding number expansion we have

$$\det M(U,\phi)_{n=1} = e^{A_0 + A_1\cos(\phi+\delta_1)}. \tag{4.5}$$

The Fourier transform can now be computed analytically; we have

$$\int_0^{2\pi} \frac{d\phi}{2\pi} e^{-ik\phi} e^{A_0 + A_1\cos(\phi+\delta_1)} = e^{A_0 + ik\delta_1} \mathrm{I}_k(A_1), \tag{4.6}$$

where I_k is Bessel function of the first kind.

For higher orders in the winding number expansion, we compute the Fourier transform using the Taylor expansion:

$$\begin{aligned}
&\int_0^{2\pi}\frac{d\phi}{2\pi}e^{-ik\phi}e^{A_0+A_1\cos(\phi+\delta_1)}e^{A_2\cos(2\phi+\delta_2)+A_3\cos(3\phi+\delta_3)+\ldots}\\
&=\int_0^{2\pi}\frac{d\phi}{2\pi}e^{-ik\phi}e^{A_0+A_1\cos(\phi+\delta_1)}(1+A_2\cos(2\phi+\delta_2)+\frac{1}{2!}A_2^2\cos(2\phi+\delta_2)^2+\ldots)\times\\
&\quad(1+A_3\cos(3\phi+\delta_3)+\frac{1}{2!}A_3^2\cos(3\phi+\delta_3)^2+\ldots)\times\ldots\\
&=c_{00}\mathrm{I}_k(A_1)+c_{+01}\mathrm{I}_{k+1}(A_1)+c_{-01}\mathrm{I}_{k-1}(A_1)+c_{+02}\mathrm{I}_{k+2}(A_1)+c_{-02}\mathrm{I}_{k-2}(A_1)+\ldots \qquad (4.7)
\end{aligned}$$

In leading to the final result in Eq. (4.7), we have used the property that $\cos(n\phi+\delta_n)=[e^{i(n\phi+\delta_n)}+e^{-i(n\phi+\delta_n)}]/2$ and the Fourier transform with two exponentials, according to Eq. (4.6), gives the Bessel functions $I_{k\pm n}(A_1)$. The coefficients c_{00},c_{+0n},c_{-0n} are the sum of terms for the Bessel functions $I_k(A_1),I_{k=1}(A_1),I_{k-n}(A_1)$.

Using Eq. (4.7) and the recursion relation for the Bessel function, $\mathrm{I}_{k-1}(A)=\frac{2k}{A}\mathrm{I}_k(A)+\mathrm{I}_{k+1}(A)$, the winding number expansion can be extended easily to higher orders.

5. Numerical tests

As we mentioned before, the success of the method rests on the assumption that we can get a very good approximation of the exponent using only a few terms in the Fourier expansion. In Fig. 2, in the top row we plot $\mathrm{Tr}\log M(\phi)$ evaluated at 204 different values of ϕ in the interval $[0,2\pi]$ (the three plots are the same); the second row shows an approximation using 1, 3 and 6 terms respectively. It is easy to see that the approximations are all very good – this is due to the fact that the first term in the expansion is much larger than the subsequent terms. To see the contributions of the higher terms in the third row, we plot the difference between the exact value (top row) and the approximation (second row). It is easy to see that the error of the approximation decreases very rapidly with the number of terms. Note also that the error is well described by a cosine function: this is due to the fact that the Fourier coefficients A_n decrease exponentially with increasing n. The error will be dominated by the first term that is not included in the approximation: A_2 for the first column, A_4 for the second and A_7 for the third.

For our tests we decided to keep a winding number expansion to the sixth order. From Fig. 2 it is easy to see that the error introduced by this approximation is of the order of 10^{-7} which is precise enough for our purposes. It is important to note that to determine the coefficients A_n exactly we would need to evaluate $\log\det M(U,\phi)$ for all possible values of ϕ. However, we can approximate their values using a discrete Fourier transform. To determine the right number of points N_d for the discrete ϕ_i needed, we compute these coefficients using an increasing number of N_d. In Table 2 we present the coefficients determined for a particular configuration; it is easy to see that $N_d=16$ is good enough to determine the coefficients with sufficient precision for our purpose.

The final test, and the most important, is to determine how accurate this approximation is when computing the projected determinant. In Fig. 3 we compare the result of this approximation with a high order approximation that uses the simple discrete Fourier transform. The expectation is that as we increase the number of quarks the value of the projected determinant decreases exponentially. It

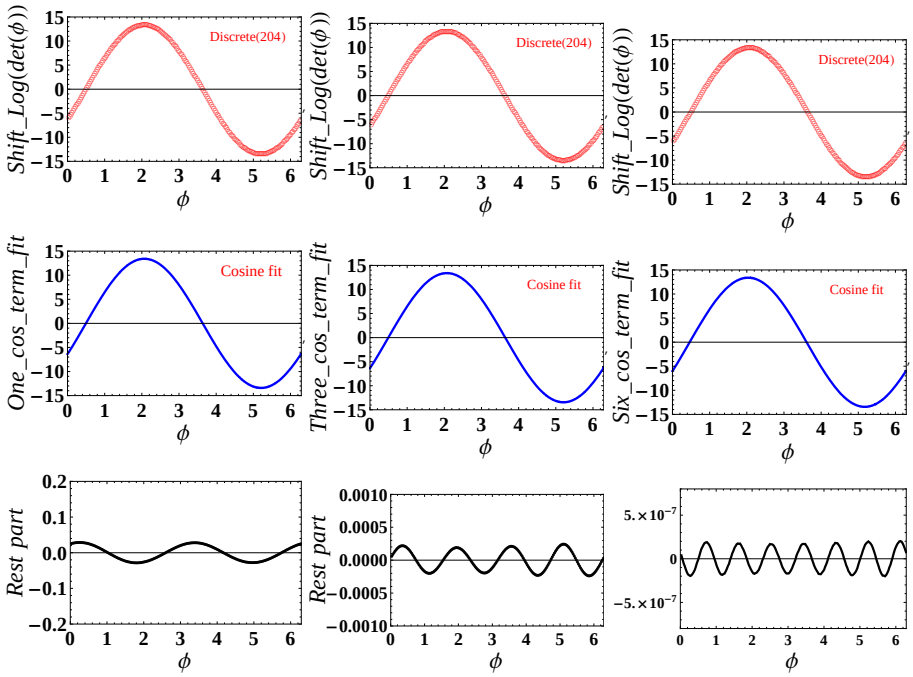

Figure 2: A comparison between the exact value for $\log\det M(U,\phi)$ and its winding number expansion to various orders. The value of $\log\det M(U,\phi)$ is shifted so that it averages to zero.

	Nd=16	Nd=24	Nd=36	Nd=200
A0	2.357308E+02	2.357308E+02	2.357308E+02	2.357308E+02
A1	-1.341400E+01	-1.341400E+01	-1.341400E+01	-1.341400E+01
A2	2.820535E-02	2.820535E-02	2.820535E-02	2.820535E-02
A3	4.135219E-04	4.135043E-04	4.134942E-04	4.134755E-04
A4	2.148188E-04	2.147950E-04	2.147792E-04	2.147547E-04
A5	2.641758E-05	2.639153E-05	2.637794E-05	2.636227E-05
A6	2.289491E-06	2.286772E-06	2.291285E-06	2.305249E-06

Table 2: The expansion coefficients determined using a discrete Fourier transform.

is easy to see that this is indeed the case for all approximations at low quark number, say for $k \leq 6$. However, as the quark number gets close to 30 the projected determinant calculated from the old approximation (the red points) flattens out – this is the onset of numerical instability. The new approximation method doesn't suffer from this problem and the projected determinant continues to decrease as the quark number is increased. We note that the winding number expansion method (WNEM) approximates well the results from the high precision discrete Fourier transform ($N_d = 204$) in its stability range. We conclude that the WNEM approximation is stable and accurate for a much larger range of quark number projection.

From Fig. 3 we also note that, as concluded above, to determine the coefficients A_n with enough precision, we don't need to use a high order approximation. Both the curves WNEM(16) and WNEM(204) with $N_d = 16$ and 204 respectively are determined using a 6^{th} order WNEM. The only difference is the set of coefficients used: WNEM(16) uses the coefficients appearing in the

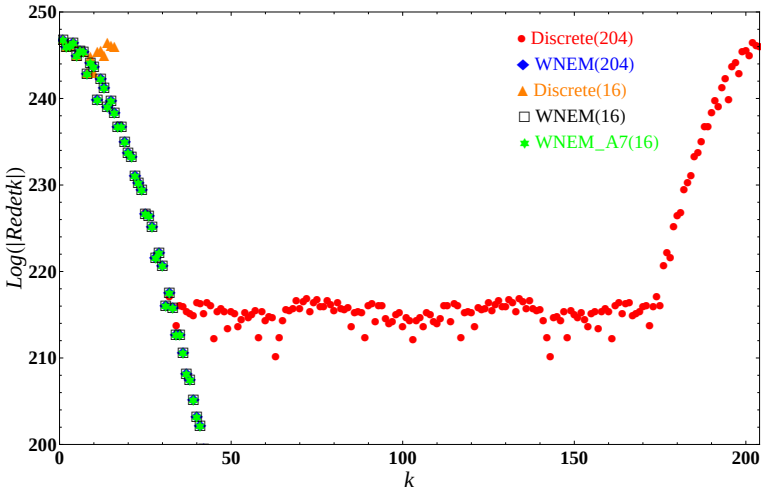

Figure 3: The projected determinant as a function of the quark number. We plot here the results of various approximation based on either the discrete Fourier transform or on the winding number expansion.

first column in Table 2, while WNEM(204) uses the coefficients in the last column. We find that the resultant projected determinants differ only by 10^{-6} in relative errors for the quark number k up to 50. This is very important since it allows us to speed up the calculation tremendously without losing precision.

To compare the merits of the WNEM with the discrete Fourier transform, we compute the values of the projected determinant calculated from the discrete Fourier transform with $N_d = 16$ only. In Fig.2 these results are labeled Discrete(16). It is easy to see that this approximation is only valid up to $k = 6$. This is to be compared to WNEM(16) that takes the same computational time but can approximate the projected determinant for $k = 40$ and beyond.

One final test was to compare the 6^{th} order WNEM with the 7^{th} order WNEM. The results are plotted in Fig. 2. The relative error between the two is less than 10^{-4} for k up to 50. We conclude that a 6^{th} order WNEM using $N_d = 16$ is precise enough for the simulations for the present lattice ($6^3 \times 4$ at $\beta = 5.2$ and quark mass $\kappa = 0.158$).

6. Conclusion

In this paper we discussed a novel approximation method for the projected determinant. The original approximation that employs a discrete Fourier transform becomes numerically unstable at large quark numbers which limits the region of the phase space that can be studied using the canonical approach. We find that our method based on the winding number expansion is numerically stable and much faster which allows us to study higher baryon numbers.

The winding number expansion method has been used successfully to carry out finite density simulations for QCD with two and four degenerate quark flavors [4]. Our numerical checks show that for all these ensembles the approximation is accurate.

Finally, we should mention that the conclusions we have drawn in this paper are valid for the fairly heavy quark mass we used ($m_\pi \sim 1$GeV). As the quark mass is lowered, we expect that more terms of A_n will be needed in the expansion.

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