A Finite Baryon Density Algorithm

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I will review the progress toward a finite baryon density algorithm in the canonical ensemble approach which entails particle number projection from the fermion determinant. These include an efficient Padé-$Z_2$ stochastic estimator of the $Tr \log$ of the fermion matrix and a Noisy Monte Carlo update to accommodate unbiased estimate of the probability. Finally, I will propose a Hybrid Noisy Monte Carlo algorithm to reduce the large fluctuation in the estimated $Tr \log$ due to the gauge field which should improve the acceptance rate. Other application such as treating $u$ and $d$ as two separate flavors is discussed.

1 Introduction

Finite density is a subject of keen interest in a variety of topics, such as nuclear equation of state, neutron stars, quark gluon plasma and color superconductivity in nuclear physics and astrophysics, and high temperature superconductors in condensed matter physics. Despite recent advance with small chemical potential at finite temperature \cite{1}, the grand canonical approach with chemical potential remains a problem for finite density at zero temperature.

The difficulty with the finite chemical potential in lattice QCD stems from the infamous sign problem which impedes important sampling with positive probability. The partition function for the grand canonical ensemble is represented by the Euclidean path-integral

$$Z_{GC}(\mu) = \int D Ud \det M[U, \mu] e^{-S_g[U]}, \quad (1)$$

where the fermion fields with fermion matrix $M$ has been integrated to give the determinant. $U$ is the gauge link variable and $S_g$ is the gauge action. The

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chemical potential is introduced to the quark action with the $e^{\mu a}$ factor in the time-forward hopping term and $e^{-\mu a}$ in the time-backward hopping term. Here $a$ is the lattice spacing. However, this causes the fermion action to be non-$\gamma_5$-Hermitian, i.e. $\gamma_5 M \gamma_5 \neq M^\dagger$. As a result, the fermion determinant $det M[U]$ is complex that leads to the sign problem.

2 Finite Chemical Potential

There are several approaches to avoid the sign problem. It was proposed by the Glasgow group \cite{2} that the sign problem can be circumvented based on the expansion of the grand canonical partition function in powers of the fugacity variable $e^{\mu/T}$,

$$Z_{GC}(\mu/T, T, V) = \sum_{B=-3V}^{B=3V} e^{\mu/T B} Z_B(T, V), \quad (2)$$

where $Z_B$ is the canonical partition function for the baryon sector with baryon number $B$. $Z_{GC}$ is calculated with reweighting of the fermion determinant. Since $Z_{GC}(\mu/T, T, V)$ is calculated with reweighting based on the gauge configuration with $\mu = 0$, it avoids the sign problem. However, this does not work, except perhaps for small $\mu$ near the finite temperature phase transition. We will dwell on this later in Sec. 3. This is caused by the ‘overlap problem’ \cite{3} where the important samples of configurations in the $\mu = 0$ simulation has exponentially small overlap with those relevant for the finite density. To alleviate the overlap problem, a reweighting in multi-parameter space is proposed \cite{4} and has been applied to study the end point in the $T-\mu$ phase diagram. In this case, the Monte Carlo simulation is carried out where the parameters in the set $\alpha_0$ include $\mu = 0$ and $\beta_c$ which corresponds to the phase transition at temperature $T_c$. The parameter set $\alpha$ in the reweighted measure include $mu \neq 0$ and an adjusted $\beta$ in the gauge action. The new $\beta$ is determined from the Lee-Yang zeros so that one is following the transition line in the $T-\mu$ plane and the large change in the determinant ratio in the reweighting is compensated by the change in the gauge action to ensure reasonable overlap. This is shown to work to locate the transition line from $\mu = 0$ and $T = T_c$ down to the critical point on the $4^4$ and $6^3 \times 4$ lattices with staggered fermions \cite{4}.

While the multi-parameter reweighting is successful near the transition line, it is not clear how to extend it beyond this region, particularly the $T=0$ case where one wants to keep the $\beta$ and quark mass fixed while changing the $\mu$. One still expects to face the overlap problem in the latter case. It is shown \cite{5} that Taylor expanding the observables and the rewriting factor leads to coefficients expressed in local operators and thus admits study of larger volumes, albeit still with small $\mu$ at finite temperature.

In the imaginary chemical potential approach, the fermion determinant is real and one can avoid the sign problem \cite{6, 7, 8, 9}. In practice, a reference imaginary chemical potentials is used to carry out the Monte Carlo
calculation and the determinants at other chemical potential values are calculated through a bosonic Monte Carlo calculation so that one can obtain the finite baryon partition function $Z_B(T, V)$ through the Fourier transform of the grand canonical partition function $Z_{GC}(\mu/T, T, V)$ [8]. However, this is problematic for large systems when the determinant cannot be directly calculated and it still suffers from the overlap problem. The QCD phase diagram has been studied with physical observables Taylor expanded and analytically continued to the real $\mu$ [9]. Again, due to the overlap problem, one is limited to small real $\mu$ near the finite temperature phase transition.

3 Finite Baryon Density – A Canonical Ensemble Approach

An algorithm based on the canonical ensemble approach to overcome the overlap problem at zero temperature is proposed [10]. To avoid the overlap problem, one needs to lock in a definite nonzero baryon sector so that the exponentially large contamination from the zero-baryon sector is excluded. To see this, we first note that the fermion determinant is a superposition of multiple quark loops of all sizes and shapes. This can be easily seen from the property of the determinant

$$\det M = e^{Tr \log M} = 1 + \sum_{n=1}^{\infty} \frac{(Tr \log M)^n}{n!}. \quad (3)$$

Upon a hopping expansion of $\log M$, $Tr \log M$ represents a sum of single loops with all sizes and shapes. The determinant is then the sum of all multiple loops. The fermion loops can be separated into two classes. One is those which do not go across the time boundary and represent virtual quark-antiquark pairs; the other includes those which wraps around the time boundary which represent external quarks and antiquarks. The configuration with a baryon number one which contains three quark loops wrapping around the time boundary will have an energy $M_B$ higher than that with zero baryon number. Thus, it is weighted with the probability $e^{-M_B N_t a_t}$ compared with the one with no net baryons. We see from the above discussion that the fermion determinant contains a superposition of sectors of all baryon numbers, positive, negative and zero. At zero temperature where $M_B N_t a_t \gg 1$, the zero baryon sector dominates and all the other baryon sectors are exponentially suppressed. It is obvious that to avoid the overlap problem, one needs to select a definite nonzero baryon number sector and stay in it throughout the Markov chain of updating gauge configurations. To select a particular baryon sector from the determinant can be achieved by the following procedure [11]: first, assign an $U(1)$ phase factor $e^{-i\phi}$ to the links between the time slices $t$ and $t+1$ so that the link $U/U^\dagger$ is multiplied by $e^{-i\phi}/e^{i\phi}$; then the particle number projection can be carried out through the Fourier transformation of the fermion determinant like in the BCS theory.
\[ P_N = \frac{1}{2\pi} \int_0^{2\pi} d\phi e^{-i\phi N} \det M[\phi] \]  

(4)

where \( N \) is the net quark number, i.e. quark number minus antiquark number. Note that all the virtual quark loops which do not reach the time boundary will have a net phase factor of unity; only those with a net \( N \) quark loops across the time boundary will have a phase factor \( e^{i\phi N} \) which can contribute to the integral in Eq. (4). Since QCD in the canonical formulation does not break \( Z(3) \) symmetry, it is essential to take care that the ensemble is canonical with respect to triality. To this end, we shall consider the triality projection \[ \text{det}_0 M = \frac{1}{3} \sum_{k=0,\pm 1} \det M[\phi + k2\pi/3]. \]  

(5)

This amounts to limiting the quark number \( N \) to a multiple of 3. Thus the triality zero sector corresponds to baryon sectors with integral baryon numbers.

\[ 8^3 \times 12 \ \beta = 6.0 \ \kappa = 0.150 \text{ Wilson action lattice} \]

![Fig. 1. \( Tr \log M[\phi] \) for a \( 8^3 \times 12 \) configuration with Wilson action as a function of \( \phi \).](image)

Another essential ingredient to circumvent the overlap problem is to stay in the chosen nonzero baryon sector so as to avoid mixing with the zero baryon sector with exponentially large weight. This can be achieved by preforming
the baryon number projection as described above before the accept/reject step in the Monte Carlo updating of the gauge configuration. If this is not done, the accepted gauge configuration will be biased toward the zero baryon sector and it is very difficult to project out the nonzero baryon sector afterwards. This is analogous to the situation in the nuclear many-body theory where it is known \[13\] that the variation after projection (Zeh-Rouhaninejad-Yoccoz method \[14,\ 15\]) is superior than the variation before projection (Peierls-Yoccoz method \[16\]). The former gives the correct nuclear mass in the case of translation and yields much improved wave functions in mildly deformed nuclei than the latter.

To illustrate the overlap problem, we plot in Fig. 1 \( Tr \log M[\phi] \) for a configuration of the \( 8^3 \times 12 \) lattice with the Wilson action at \( \beta = 6.0 \) and \( \kappa = 0.150 \) which is obtained with 500 \( Z_2 \) noises. We see that the it is rather flat in \( \phi \) indicating that the Fourier transform in Eq. (4) will mainly favor the zero baryon sector. On the other hand, at finite temperature, it is relatively easier for the quarks to be excited so that the zero baryon sector does not necessarily dominate other baryon sectors. Another way of seeing this is that the relative weighting factor \( e^{-M_B N_{\alpha \tau}} \) can be \( O(1) \) at finite temperature. Thus, it should be easier to project out the nonzero baryon sector from the determinant. We plot in Fig. 2 a similarly obtained \( Tr \log M[\phi] \) for configuration of the \( 8 \times 20^2 \times 4 \) lattice at finite temperature with \( \beta = 4.9 \) and \( \kappa = 0.182 \). We see from the figure that there is quite a bit of wiggling in this case as compared
to that in Fig. 1. This implies that it is easier to project out a nonzero baryon sector through the Fourier transform at finite temperature.

4 Noisy Monte Carlo with Fermion Determinant

In order to implement the canonical ensemble approach, it is clear that one needs to evaluate the fermion determinant for the purpose of particle projection. Since the pseudofermion approach does not give the determinant in the Markov process, it is not applicable. In view of the fact that it is impractical to calculate the determinant directly for realistic volumes, a Monte Carlo algorithm which accommodates an unbiased estimate of the probability and an efficient way to estimate the determinant are necessary for the finite baryon density calculation.

A noisy Monte Carlo algorithm [17] with Padé-Z estimates [18, 19] of the $T r \log$ of the fermion matrix are developed toward this goal and a numerical simulation with Wilson dynamical fermion is carried out [20]. We shall summarize the progress made so far.

The QCD partition function can be written in the form

$$Z = \int dU \ e^{-S_g(U)} \int \prod_{i=1}^{\infty} d\eta_i \ P^\eta(\eta_i) \times \prod_{k=2}^{\infty} d\rho_k \ P^\rho(\rho_k) \ f(U, \eta, \rho),$$

where $S_g(U)$ is the gauge action. $f(U, \eta, \rho)$ stands for $f(U, \{\eta_i\}, \{\rho_k\})$ which is an unbiased stochastic estimator [21] of the fermion determinant $e^{Tr \log M}$ via an infinite number of auxiliary variables $\rho_k$ and $\eta_i$. $P^\eta(\eta_i) = \delta(\eta_i - 1)$ is the distribution for the $Z_2$ noise $\eta_i$ and $P^\rho(\rho_k) = \theta(\rho_k) - \theta(\rho_k - 1)$ is the flat distribution for $0 \leq \rho_k \leq 1$. With $f(U, \{\eta_i\}, \{\rho_k\})$ being the stochastic expansion

$$f(U, \{\eta_i\}, \{\rho_k\}) = 1 + \left\{ x_1 + \theta(1 - \rho_2) \left\{ x_2 + \theta \left( \frac{1}{3} - \rho_3 \right) \left\{ x_3 + \ldots \right. \right. \right. \right.$$

$$\left. \left. \right. \left. \left. \left. \ldots + \theta \left( \frac{1}{n} - \rho_n \right) \left\{ x_n + \ldots \right\} \right\} \right\} \left\} \right\},$$

where $x_i = \eta_i^\dagger \ln M(U) \eta_i$, one can verify [21] that

$$\prod_{i=1}^{\infty} d\eta_i \ P^\eta(\eta_i) \prod_{k=2}^{\infty} d\rho_k \ P^\rho(\rho_k) \langle f(U, \{\eta_i\}, \{\rho_k\}) \rangle = e^{Tr \ln M(U)},$$

and the stochastic series terminates after $e$ terms on the average.
Since the estimator $f(U, \eta, \rho)$ can be negative due to the stochastic estimation, the standard treatment is to absorb the sign into the observables, i.e.

$$\langle O \rangle_P = \frac{\langle O \text{ sgn}(P) \rangle_{\langle |P| \rangle}}{\langle \text{ sgn}(P) \rangle_{\langle |P| \rangle}}.$$  (9)

With the probability for the gauge link variable $U$ and noise $\xi \equiv (\eta, \rho)$ written as $P(U, \xi) \propto P_1(U)P_2(U, \xi)P_3(\xi)$ with

$$P_1(U) \propto e^{-S_g(U)}$$
$$P_2(U, \xi) \propto |f(U, \xi)|$$
$$P_3(\xi) \propto \prod_{i=1}^{\infty} P^{\eta}(\eta_i) \prod_{k=2}^{\infty} P^{\rho}(\rho_k),$$  (10)

the following two steps are needed to prove detailed balance [17, 20].

(a) Let $T_1(U, U')$ be the ergodic Markov matrix satisfying detailed balance with respect to $P_1$, in other words $P_1(U)T_1(U, U')dU = P_1(U')T_1(U', U)dU'$. Then the transition matrix

$$T_{12}(U, U') = T_1(U, U') \min \left[1, \frac{P_2(U', \xi)}{P_2(U, \xi)} \right]$$  (11)

satisfies detailed balance with respect to the $P_1(U)P_2(U, \xi)$ (with $\xi$ fixed).

(b) The transition matrix

$$T_{23}(\xi, \xi') = P_3(\xi') \min \left[1, \frac{P_2(U', \xi')}{P_2(U, \xi)} \right]$$  (12)

satisfies detailed balance with respect to $P_2(U, \xi)P_3(\xi)$ (with $U$ fixed).

From (a), (b) it follows that $T_{12}$ and $T_{23}$ keep the original distribution $P(U, \xi)$ invariant and interleaving them will lead to an ergodic Markov process with the desired fixed point.

4.1 Padé - Z_2 Estimator of Tr ln M with Unbiased Subtraction

In Eq. (7), one needs to calculate $x_i = \eta_i \ln M(U)\eta_i$ in the stochastic series expansion of the fermion determinant. An efficient method is developed to calculate it [18]. First of all, the logarithm is approximated using a Padé approximation, which after the partial fraction expansion, has the form

$$\ln M(U, \kappa) \approx R_M(U) \equiv b_0 I + \sum_{i=1}^{N_P} b_i (M(U, \kappa) + c_i I)^{-1}$$  (13)

where $N_P$ is the order of the Padé approximation, and the constants $b_i$ and $c_i$ are the Padé coefficients. In our implementation we have used an 11-th
order approximation whose coefficients are tabulated in [18]. The traces of \( \ln M \) are then estimated by evaluating bilinears of the form \( \eta^\dagger R_M(U) \eta \). If the components of \( \eta \) are chosen from the complex \( \mathbb{Z}_2 \) group, then the contributions to the variance of these bilinears come only from off diagonal elements of \( R_M(U) \) \[ 22, 19 \]. In this sense, \( \mathbb{Z}_2 \) noise is optimal and has been applied to the calculation of nucleon matrix elements involving quark loops [23]. A n effective method reducing the variance is to subtract off a linear combination of traceless operators from \( R_M(U) \) and to consider

\[
E[\text{Tr} R_M(U), \eta] = \eta^\dagger (R_M(U) - \alpha_i O_i) \eta . \tag{14}
\]

Here the \( O_i \) are operators with \( \text{Tr} O_i = 0 \). Clearly since the \( O_i \) are traceless they do not bias the estimators. The \( \alpha_i \) are constants that can be tuned to minimize the fluctuations in \( E[\text{Tr} R_M(U), \eta] \).

With other types of noise such as Gaussian noise, the variance receives contributions from diagonal terms which one cannot subtract off. In this case, the unbiased subtraction scheme described here is ineffective. In practice, the \( O_i \) are constructed by taking traceless terms from the hopping parameter expansion for \( M^{-1}(U) \). It is shown for Wilson fermions on a \( 8^3 \times 12 \) lattice at \( \beta = 5.6 \), these subtractions can reduce the noise coming from the terms \((M(U) + c_1)^{-1}\) in equation [18] by a factor as large as 37 for \( \kappa = 0.150 \) with 50 \( \mathbb{Z}_2 \) noises [18].

### 4.2 Implementation of the Noisy Monte Carlo Algorithm

The noisy Monte Carlo algorithm has been implemented for the Wilson dynamical fermion with pure gauge update (Kentucky Noisy Monte Carlo Algorithm) for an \( 8^4 \) lattice with \( \beta = 5.5 \) and \( \kappa = 0.155 \) [20]. Several tricks are employed to reduce the fluctuations of the \( \text{Tr} \ln M \) estimate and increase the acceptance. These include shifting the \( \text{Tr} \ln M \) with a constant, \( \Delta \beta \) shift [24], and splitting the \( \text{Tr} \ln M \) with \( N \) ‘fractional flavors’. After all these efforts, the results are shown to agree with those from the HMC simulation. However, the autocorrelation is very long and the acceptance rate is low. This has to do with the fact that \( \text{Tr} \ln M \) is an extensive quantity which is proportional to volume and the stochastic series expansion of \( e^x \) converges for \( x \leq 6 \) for a sample with the size of \( \sim 10^3 - 10^4 \). This is a stringent requirement which requires the fractional flavor number \( N \geq 15 \) for this lattice. This can be seen from the distribution of \( x = \sum \lambda (\text{Tr}R_M^f(U) - M^f \text{Plag} - x_0^f) / N \) in Fig. 3 which shows that taking \( N \) to be 15, 20, and 25, the largest \( x \) value is less than 6.

As the volume increases, this fractional flavor needs to be larger to keep \( x \) smaller than 6 for a sample of the size \( \sim 10^3 - 10^4 \). At the present volume \( (8^4) \), the autocorrelation is already much longer than that of HMC, it is going to be even less efficient for larger volumes. This is generic for the noisy Monte Carlo algorithm which scale with volume as \( V^2 \), while HMC scales as \( V^{5/4} \).
5 Hybrid Noisy Monte Carlo Algorithm – a New Proposal

It is clear that the inefficiency of the noisy Monte Carlo algorithm for the fermion determinant is due to the large fluctuation of the $Tr \ln M$ estimator from one gauge configuration to the next. We shall propose a combined Hybrid Monte Carlo (HMC) and Noisy Monte Carlo (NMC) to remove such fluctuations in the context of the finite density.

With the baryon number projection discussed in Sec. 3, we can write the partition function for the finite baryon sector with $B$ baryons as

$$Z_B = \int dp d\phi^2 d\phi e^{-p^2/2-S_{\phi}(U)+\phi^T (M^\dagger M)^{-1} \phi} \frac{\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-i3B\theta} det M^\dagger M[\theta]}{det M^\dagger M[\theta = 0]}.$$  \hspace{1cm} (15)

In this case, one can update the momentum $p$, the gauge link variable $U$ and the pseudofermion field $\phi$ via HMC and then interleave with NMC for updating the determinant ratio

$$R = \frac{\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-i3B\theta} det M^\dagger M[\theta]}{det M^\dagger M[\theta = 0]}.$$  \hspace{1cm} (16)

As described in Sec. 4, NMC involves two Metropolis accept/reject steps to update the ratio with the Padé - $Z_2$ estimator of the $Tr \ln$ difference of the determinants, i.e. $Tr(\ln M^\dagger M[\theta] - \ln M^\dagger M[\theta = 0])$. It is pointed out [25]...
that for zero temperature, one can approximate the continuous integral over $\theta$ with a discrete sum incorporating triality zero projection \[11, 12\] so that the partition function is a mixture of different $Z_B$ for different baryon number $B$. In other words, the approximation

$$\frac{1}{2\pi} \int_0^{2\pi} d\theta e^{-i3B\theta} \det M^\dagger M[\theta] \rightarrow \frac{1}{3B_N} \sum_{k=0}^{3B_N-1} e^{-i\frac{2\pi kB}{3B_N}} \det M^\dagger M[\frac{2\pi kB}{3B_N}]$$

(17)

leads to the mixing of the baryon sector $B$ with those of $B \pm B_N, B \pm 2B_N, \ldots$. For example, if we take $B = 1$ and $B_N = 5$, the discrete approximation gives an admixture of partition function with baryon number $B = 1, 5, 11, -4, -9, \ldots$. At zero temperature, the partition function $Z_B$ behaves like $e^{-Bm_NN_{\text{lat}}}$, one expects that the mixing due to baryons other than $B = 1$ will be exponentially suppressed when $m_NN_{\text{lat}} > 1$.

Two points need to be stressed. First of all, it is crucial to project out the particle number in Eq. (17) before the Metropolis accept/reject step in order to overcome the overlap problem. Secondly, given that the ratio $R$ in Eq. (16) is replaced with a discrete sum

$$\overline{R} = \frac{1}{3B_N} \sum_{k=0}^{3B_N-1} e^{-i\frac{2\pi kB}{3B_N}} e^{\text{Tr} \ln M^\dagger M[\frac{2\pi kB}{3B_N}] - \ln M^\dagger M[0]}$$

(18)

which involves the difference between the $\text{Tr} \ln M^\dagger M[\frac{2\pi kB}{3B_N}]$ and $\text{Tr} \ln M^\dagger M[0]$, it takes out the fluctuation due to the gauge configuration which plagued the Kentucky Noisy Monte Carlo simulation in Sec. 4. Furthermore, the $\text{Tr} \ln$ difference is expected to be $O(1)$ as seen from Fig. 1. If indeed is the case, it should lead to a better convergence of the stochastic series expansion in Eq. (7) and the algorithm scales with volume the same as HMC.

5.1 Another Application

Here we consider another possible application of the Hybrid Noisy Monte Carlo algorithm. HMC usually deals with two degenerate flavors. However, nature comes with 3 distinct light flavors – $u, d$ and $s$. To consider $u$ and $d$ as separate flavors, one can perform HMC with two degenerate flavors at the $d$ quark mass and then employ NMC to update the determinant ratio

$$R_{ud} = \frac{\text{Det}M_u^\dagger \text{Det}M_d}{\text{Det}M_d^\dagger \text{Det}M_u} = e^{\text{Tr}(\ln M_u - \ln M_d)}.$$  

(19)

Since both the $u$ and $d$ masses are much smaller than $\Lambda_{QCD}$, $\text{Tr}(\ln M_u - \ln M_d)$ should be small. If the $\text{Tr} \ln$ difference is small enough (e.g. $O(1)$) so that the acceptance rate is high, it could be a feasible algorithm for treating $u$ and $d$
as distinct flavors so that realistic comparison with experiments can be done someday. It is shown recently that the Rational Hybrid Monte Carlo Algorithm (RHMC) \cite{26, 27} works efficiently for two flavor staggered fermions. It can be applied to single flavors for Wilson, domain wall, or overlap fermions at the cost of one pseudofermion for each flavor. We should point out that, in comparison, the Hybrid Noisy approach discussed here saves one pseudofermion, but at the cost of having to update the determinant ratio $R_{\text{ud}}$ in Eq. (19).

While we think that the Hybrid Noisy Monte Carlo algorithm proposed here might overcome the overlap and the low acceptance problems and the determinant $\det M[\theta]$ is real in this approach, the fact that the Fourier transform in Eq. (17) involves the baryon number $B$ may still lead to a sign problem in the thermodynamic limit when $B$ and $V$ are large. However, as an initial attempt, we are more interested in finding out if the algorithm works for a small $B$ such as 1 or 2 in a relatively small box.

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