FACTORIZATION METHOD FOR SIMULATING QCD AT FINITE DENSITY

JUN NISHIMURA*
Department of Physics, Nagoya University,
Nagoya 464-8602, Japan
E-mail: nisimura@eken.phys.nagoya-u.ac.jp

We propose a new method for simulating QCD at finite density. The method is based on a general factorization property of distribution functions of observables, and it is therefore applicable to any system with a complex action. The so-called overlap problem is completely eliminated by the use of constrained simulations. We test this method in a Random Matrix Theory for finite density QCD, where we are able to reproduce the exact results for the quark number density.

1. Introduction
Recently there are a lot of activities in QCD at finite density, where interesting phases such as a superconducting phase have been conjectured to appear\(^1\). At zero chemical potential Monte Carlo simulations of lattice QCD enables nonperturbative studies from first principles. It is clearly desirable to extend such an approach to finite density and explore the phase diagram of QCD in the \(T\)(temperature)-\(\mu\)(chemical potential) plane. The main obstacle is here that the Euclidean action becomes complex once the chemical potential is switched on.

Nevertheless QCD at finite density has been studied by various approaches with exciting conjectures. First there are perturbative studies which are valid in the \(\mu \to \infty\) limit\(^2\).\(^3\). Refs. [4] and [5] uses effective theories with instanton-induced four-fermi interactions. As for Monte Carlo studies two directions have been pursued so far. One is to modify the model so that the action becomes real. This includes changing the gauge group\(^6\) from SU(3) to SU(2), and introducing a chemical potential with opposite signs for up and down quarks\(^7\). The other direction is to explore

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\*Work partially supported by Grant-in-Aid for Scientific Research (No. 14740163) from the Ministry of Education, Culture, Sports, Science and Technology.
the large $T$ and small $\mu$ regime of lattice QCD, where the imaginary part of the action is not very large. These studies already produced results relevant to heavy ion collision experiments, but more interesting physics will be uncovered if larger $\mu$ regime becomes accessible by simulations.

In Ref. [10] we have proposed a new method to simulate systems with a complex action, which utilizes a simple factorization property of distribution functions of observables. Since the property holds quite generally, the approach can be applied to any system with a complex action. The most important virtue of the method is that it eliminates the so-called overlap problem, which occurs in the standard re-weighting method. Ultimately we hope that this method will enable us, among other things, to explore the phase diagram of QCD at finite baryon density. As a first step we have tested the new approach in a Random Matrix Theory for finite density QCD, which can be regarded as a schematic model for QCD at finite baryon density.

2. Random Matrix Theory for finite density QCD

The Random Matrix Model we study is defined by the partition function

$$Z = \int dW e^{-N \text{tr}(W^\dagger W)} \det D ,$$

where $W$ is a $N \times N$ complex matrix, and $D$ is a $2N \times 2N$ matrix given by

$$D = \begin{pmatrix} m & iW + \mu \\ iW^\dagger + \mu & m \end{pmatrix} .$$

The parameters $m$ and $\mu$ correspond to the ‘quark mass’ and the ‘chemical potential’, respectively. In what follows we consider the massless case ($m = 0$) for simplicity and we focus on the ‘quark number density’ defined by

$$\nu = \frac{1}{2N} \text{tr} (\gamma_4 D^{-1}) , \quad \gamma_4 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} .$$

The vacuum expectation value (VEV) of the quark number density is obtained exactly by [13] and in particular in the large-$N$ limit

$$\lim_{N \to \infty} \langle \nu \rangle = \begin{cases} -\mu & \text{for } \mu < \mu_c \\ \frac{1}{\mu} & \text{for } \mu > \mu_c \end{cases},$$

where $\mu_c$ is the solution to the equation $1 + \mu^2 + \ln(\mu^2) = 0$, and its numerical value is given by $\mu_c = 0.527 \cdots$. We find that the quark number density $\langle \nu \rangle$ has a discontinuity at $\mu = \mu_c$. Thus the schematic model reproduces qualitatively the first order phase transition expected to occur in ‘real’ QCD at nonzero baryon density.
3. The complex action problem

Let us first rewrite (2.1) as

\[ Z = \int dW e^{-S_0 + i \Gamma}, \]  

(3.1)

where we have introduced \( S_0 \) and \( \Gamma \) by

\[ S_0 = N \text{tr} (W^\dagger W) - \ln |\det D| \]  

(3.2)

\[ \det D = e^{i \Gamma} |\det D| . \]  

(3.3)

In this form it becomes manifest that the system has a complex action, where the problematic imaginary part \( \Gamma \) is given by the phase of the fermion determinant. Since the weight \( e^{-S_0 + i \Gamma} \) in (3.1) is not positive definite, we cannot regard it as a probability density. Hence it seems difficult to apply the idea of standard Monte Carlo simulations, which reduces the problem of obtaining VEVs to that of taking an average over an ensemble generated by the probability density.

Let us define the so-called phase quenched partition function

\[ Z_0 = \int dW e^{-N \text{tr}(W^\dagger W) - \ln |\det D|} = \int dW e^{-S_0} . \]  

(3.4)

Since the system (3.4) has a positive definite weight, the VEV \( \langle \cdot \rangle_0 \) associated with this partition function can be evaluated by standard Monte Carlo simulations. Then one can use the standard re-weighting formula

\[ \langle \nu \rangle = \frac{\langle \nu e^{i \Gamma} \rangle_0}{\langle e^{i \Gamma} \rangle_0} \]  

(3.5)

to obtain the VEV \( \langle \nu \rangle \) in the full model (3.1). The problem with this method is that the fluctuations of the phase \( \Gamma \) in (3.5) grows linearly with the size of the matrix \( D \), which is of \( O(N) \). Due to huge cancellations, both the denominator and the numerator of the r.h.s. of (3.5) vanish as \( e^{-\text{const.}N} \) as \( N \) increases, while the ‘observables’ \( e^{i \Gamma} \) and \( \nu e^{i \Gamma} \) are of \( O(1) \) for each configuration. As a result, the number of configurations required to obtain the VEVs with some fixed accuracy grows as \( e^{\text{const.}N} \).

In fact we may simplify the expression (3.5) slightly by using a symmetry. We note that the fermion determinant \( \det D \), as well as the observable \( \nu \), becomes complex conjugate under the transformation

\[ W \mapsto -W , \]  

(3.6)
while the Gaussian action remains invariant. From this we find that
\[ \langle \nu \rangle = \langle \nu_R \rangle + i \langle \nu_I \rangle = \langle \nu_R \rangle \cos \Gamma \langle \cos \Gamma \rangle_0 + i \langle \nu_I \rangle \langle \sin \Gamma \rangle_0, \]
\[ \langle \nu_R \rangle = \frac{\langle \nu_R \cos \Gamma \rangle_0}{\langle \cos \Gamma \rangle_0}; \quad \langle \nu_I \rangle = i \frac{\langle \nu_I \sin \Gamma \rangle_0}{\langle \cos \Gamma \rangle_0}, \]

where \( \nu_R \) and \( \nu_I \) denote the real part and the imaginary part of \( \nu \), respectively. This simplification, however, does not solve the problem at all, since \( \cos \Gamma \) and \( \sin \Gamma \) flip their sign violently as a function of the configuration \( W \).

Note that both terms in the r.h.s. of (3.7) are real, meaning in particular that their sum \( \langle \nu \rangle \) is also real.

The model (3.4) is solvable in the large-\( N \) limit and one obtains
\[ \lim_{N \to \infty} \langle \nu \rangle_0 = \begin{cases} \mu & \text{for } \mu < 1 \\ 1/\mu & \text{for } \mu > 1. \end{cases} \]

In this case the VEV of the quark number density is a continuous function of the chemical potential \( \mu \) unlike in (2.4). Thus the first order phase transition in the full model (3.1) occurs precisely due to the imaginary part \( \Gamma \) of the action. Note also that the symmetry under (3.6) implies
\[ \langle \nu_I \rangle_0 = 0; \quad \langle \nu_R \rangle_0 = \langle \nu \rangle_0. \]

4. The factorization method

In this section, we explain how the factorization method can be used to obtain the VEVs \( \langle \nu_R \rangle \) and \( \langle \nu_I \rangle \). The fundamental objects of the method are the distribution functions
\[ \rho_i(x) \overset{\text{def}}{=} \langle \delta(x - \nu_i) \rangle \]
\[ \rho_i^{(0)}(x) \overset{\text{def}}{=} \langle \delta(x - \nu_i) \rangle_0 \quad i = R, I \]

defined for the full model and for the phase quenched model respectively. The important property of these functions is that they factorize as
\[ \rho_i(x) = \frac{1}{C} \rho_i^{(0)}(x) \varphi_i(x) \quad i = R, I, \]
where the constant \( C \) is given by \( C \overset{\text{def}}{=} \langle e^{i \Gamma} \rangle_0 \). The ‘weight factor’ \( \varphi_i(x) \) represents the effect of \( \Gamma \), and it can be written as a VEV
\[ \varphi_i(x) \overset{\text{def}}{=} \langle e^{i \Gamma} \rangle_{i, x} \]
with respect to a yet another partition function
\[ Z_i(x) = \int dW e^{-S_0} \delta(x - \nu_i). \]
The δ-function represents a constraint on the system. In actual simulation we replace the δ-function by a sharply peaked potential. We refer the reader to Ref. [11] for the details.

Using the symmetry under (3.6), the formulae for ⟨ν⟩ is nothing but (3.8), where ⟨νR cos Γ⟩0, ⟨νI sin Γ⟩0 and ⟨cos Γ⟩0 are replaced by

\[\langle \nu_R \cos \Gamma \rangle_0 = \int_{-\infty}^{\infty} dx \ r^{(0)}_R(x) \ w_R(x), \tag{4.6}\]
\[\langle \nu_I \sin \Gamma \rangle_0 = 2 \int_{0}^{\infty} dx \ r^{(0)}_I(x) \ w_I(x), \tag{4.7}\]
\[\langle \cos \Gamma \rangle_0 = \int_{-\infty}^{\infty} dx \ r^{(0)}_R(x) \ w_R(x). \tag{4.8}\]

The weight factors \(w_i(x)\) are defined by

\[w_R(x) \equiv \langle \cos \Gamma \rangle_{R,x}; \quad w_I(x) \equiv \langle \sin \Gamma \rangle_{I,x}. \tag{4.9}\]

One of the virtues of the method can be seen from (4.6)∼(4.8). If we are to obtain the VEVs on the l.h.s. by directly simulating the system (3.4), for most of the time we sample configurations whose \(\nu_i\) takes a value close to the peak of \(r^{(0)}_i(x)\). However, from the r.h.s. of the formulae, it is clear that we have to sample configurations whose \(\nu_i\) takes a value where \(|r^{(0)}_i(x)|w_i(x)|\) becomes large, in order to obtain the VEVs accurately. In general these two regions of configuration space have little overlap, which becomes exponentially small as the system size increases. The present method resolves this ‘overlap problem’ completely by ‘forcing’ the simulation to sample the important region.

Table 1. Results of the analysis of ⟨ν⟩ described in the text. Statistical errors computed by the jackknife method are shown. The last column represents the exact result for ⟨ν⟩ at each \(\mu\) and \(N\). For \(\mu = 0.2\) the exact result is ⟨ν⟩ = −0.2 with an accuracy better than 1 part in 10−9.

| \(\mu\) | \(N\) | \(\langle \nu_R \rangle\) | \(\langle \nu_I \rangle\) | ⟨ν⟩ | ⟨ν⟩ (exact) |
|---|---|---|---|---|---|
| 0.2 | 8 | 0.0656(6) | -0.1970(5) | -0.1915(7) | -0.20000... |
| 0.2 | 16 | 0.0060(4) | -0.1905(13) | -0.1845(13) | -0.20000... |
| 0.2 | 24 | 0.0076(9) | -0.1972(14) | -0.1896(17) | -0.20000... |
| 0.2 | 32 | 0.0021(8) | -0.1947(19) | -0.1927(25) | -0.20000... |
| 0.2 | 48 | 0.0086(37) | -0.2086(54) | -0.20000(88) | -0.20000... |
| 1.0 | 8 | 0.8617(10) | 0.1981(13) | 1.0598(12) | 1.066501... |
| 1.0 | 16 | 0.8936(2) | 0.1353(6) | 1.0289(5) | 1.032240... |
| 1.0 | 32 | 0.9207(1) | 0.0945(2) | 1.0152(3) | 1.015871... |
5. Reproducing exact results by the new method

In Table 1 we show our results for two values of $\mu$, $\mu = 0.2$ and $\mu = 1.0$, which are on opposite sides of the first order phase transition point $\mu = \mu_c = 0.527 \cdots$. They are in good agreement with the exact results, and the achieved values of $N$ are large enough to extract the large $N$ limit.

Note that $\langle \nu_R \rangle \sim 0$ at $\mu = 0.2$. Thus the main contribution to $\langle \nu \rangle$ comes from the imaginary part $\langle \nu_I \rangle$, which is in sharp contrast to the results (3.10) for the phase quenched system. This result comes about because the sign change of $w_R(x)$ occurs near the peak of $\rho_R^{(0)}(x)$, so that the product $\rho_R^{(0)}(x)w_R(x)$ has a positive regime and a negative regime, which cancel each other in (4.6). For $\mu = 1.0$, on the other hand, $w_R(x)$ is approximately constant in the region where $\rho_R^{(0)}(x)$ is peaked, so the shape of the product $\rho_R^{(0)}(x)w_R(x)$ is similar to $\rho_R^{(0)}(x)$. The main contribution to $\langle \nu \rangle$ comes from the real part $\langle \nu_R \rangle$, and moreover, it is close to $\langle \nu_R \rangle_0$.

![Figure 1. The weight factor $w_R(x)$ is plotted against $x$ for $N = 8$ at various $\mu$. The behavior changes drastically as $\mu$ crosses the critical point.](image)

In Fig. 1 we plot $w_R(x)$ for $N = 8$ at various $\mu$. It is interesting that the $w_R(x)$ changes from positive to negative for $\mu < \mu_c$, but it changes from negative to positive for $\mu > \mu_c$. (Similarly $w_I(x)$ is positive at $x > 0$ for $\mu < \mu_c$, but it is negative at $x > 0$ for $\mu > \mu_c$.) Thus the behavior of $w_I(x)$
changes drastically as the chemical potential $\mu$ crosses its critical value $\mu_c$. These results provide a clear understanding of how the first order phase transition occurs due to the effects of $\Gamma$.

6. Applications to other systems with complex actions

The method \cite{14} proposed for simulating $\theta$-vacuum like systems can be regarded as a special case of the factorization method. A simplified version of the method was sufficient because the observable was identical to the imaginary part of the action. The essence of the factorization method is that it avoids the overlap problem by the use of constrained simulations. In Ref. \cite{14} promising results for 2d CP$^3$ are also reported.

In Ref. \cite{10} the method has been used to study the dynamical generation of space time in superstring theory based on its matrix model formulation \cite{15}. There the method becomes even more powerful since the distribution functions turn out to be positive definite. In this case the scaling property of the weight factor enables extrapolations to larger system size.

We hope that the factorization method is useful also for studying other interesting systems with complex actions such as Chern-Simons theories, chiral gauge theories, strongly coupled electron systems etc.

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