Lattice Study of QCD Phase Structure by Canonical Approach
– Towards determining the phase transition line

D. Boyda, V.G. Bornyakov, V. Goy, A. Molochkov, A. Nakamura, A. Nikolaev, and V. Zakharov

School of Biomedicine, Far Eastern Federal University, Russia

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We investigate the potential for using the canonical ensemble approach to determine the QCD phase diagram in the temperature - density plane. This approach allows us to study the finite baryon density regions where the well-known sign problem obstructs the standard lattice QCD numerical study. In order to make the canonical approach a reliable lattice QCD method, we perform careful error estimation, and estimate the reliable regions in real chemical potential which are related to truncation of higher canonical partition function terms, \(Z_n\). We compute the higher moments of the baryon number density including the kurtosis, and compare our results with information from relativistic heavy-ion collision experiments.

I. INTRODUCTION

Many studies have tried to reveal the properties of strongly interacting quark-gluon/hadron matter from experimental and phenomenological analyses of high-energy heavy-ion collisions [1-3]. It is expected that these studies will lead to understanding of the phase diagram in the temperature - baryon density plane, which is also looked for in cosmological research. The first principle calculations, based on lattice QCD, have a potential to provide reliable fundamental information. However, to obtain this information, we must first overcome the “sign problem”, which is described below.

The lattice QCD is a simulation study based on the grand canonical partition function,

\[
Z_{GC}(\mu, T, V) = \sum_{\{U\}} \text{det} \Delta(\mu)^{N_f} e^{-S_G}, \tag{1}
\]

where \(\mu\) is the chemical potential, \(N_f\) is flavor number, \(S_G\) is gauge part of action and \(\text{det} \Delta\) is the fermion determinant satisfying the relation

\[
(\text{det} \Delta(\mu))^* = \text{det} \Delta(-\mu^*). \tag{2}
\]

Consequently, when \(\mu\) is nonzero and real, \(\text{det} \Delta\) is complex, and when \(\mu\) is pure imaginary or zero, \(\text{det} \Delta\) is real.

In Monte Carlo simulations, the gluon fields, \(U\), are generated with the probability proportional to the integrand in Eq. (1), and therefore, if \(\text{det} \Delta\) is complex, the simulations cannot be conducted. If we separate out the phase factor, i.e. rewrite the integrand as

\[
|\text{det} \Delta| e^{i\theta} = \text{det} \Delta e^{-S_G}, \tag{3}
\]

and include only the absolute value into the probability, then the observables include the phase and oscillate. This makes the simulation practically impossible, and is called the “sign problem”.

In order to circumvent this obstacle, many approaches have been pursued; see [4] for recent review. In recent publications [5-7], where higher order cumulants were evaluated for nearly physical quark masses, mostly Taylor expansion method was employed and simulations were performed at zero chemical potential. Monte Carlo simulations for pure imaginary \(\mu\) are free from the complex measure problem, as can be seen from Eq. (2). The question is how one can extract data for real \(\mu\).

The grand canonical partition function is related to the canonical partition function, \(Z_C(n, T, V)\), as follows:

\[
Z_{GC}(\mu, T, V) = \text{Tr} \left(e^{-\frac{\hat{H} - \mu \hat{N}}{T}}\right) = \sum_{n = -\infty}^{\infty} \langle n | e^{-\frac{\hat{B}}{T}} | n \rangle e^{\frac{\mu}{T}},
\]

\[
= \sum_{n = -\infty}^{\infty} Z_C(n, T, V) e^{\frac{\mu}{T}} = \sum_{n = -n_{max}}^{n_{max}} Z_n e^{\xi n}, \tag{4}
\]

where \(\xi = e^{\mu/T}\) is the fugacity, \(\hat{N}\) is an operator of a conserved quantum number such as a baryon number or electric charge and we introduced abbreviation \(Z_n\) for \(Z_C(n, T, V)\). Here we use notation \(n_{max}\) for number of terms in the sum. Strictly speaking \(n_{max} \rightarrow \infty\), but in the real simulations we must truncate the fugacity expansion. This truncation brings some systematic error. In this report, we are mainly concerned with the baryon number case, and we write the chemical potential \(\mu_B\).

For imaginary \(\mu_B (\mu_B = i \mu_I\) and \(\theta_I = \mu I/T\), we can calculate \(Z_n\) by the inverse Fourier transformation [10] as

\[
Z_n = \int_{0}^{2\pi} \frac{d\theta_I}{2\pi} e^{-in\theta_I} Z_{GC}\left(\mu_B = i\theta_I T, T, V\right). \tag{5}
\]

Note that \(Z_n = \langle n | e^{-\hat{B}} | n \rangle \geq 0\) does not depend on \(\mu_B\), and therefore one can evaluate the grand canonical
partition function, $Z_{GC}$, in Eq. (4) for any $\mu_B$ (imaginary or real) once $Z_n$ are known. After the pioneering work of A. Hasenfratz and Toussant [11], many approaches in this direction were done [11–14].

The formula Eq. (4) is exact, and in [13], it is proven that on the finite lattice, $Z_{GC}$ is expressed as a finite series of the fugacity expansion.

Now we have a route from the imaginary to the real chemical potential regions:

- Step 1: Using Eq. (5), we calculate $Z_n$ from $Z_{GC}$ computed at the imaginary $\mu_B$.
- Step 2: Using these $Z_n$ in Eq. (4), we construct $Z_{GC}$ for the real $\mu_B$.

To search for the phase transition signals, one can use the moments $\lambda_m$, which can be also extracted from results of the heavy ion collision experiments:

$$\lambda_m(\mu_B) = \left(T \frac{\partial}{\partial \mu_B}\right)^m \log Z_{GC}.$$  

 Especially, $\lambda_2$ (susceptibility), $\lambda_3$, and $\lambda_4$, provide useful information on the phase structure. In this paper we conduct a detailed study of the canonical ensemble approach which has a potential to reveal the QCD phases. We study systematic error of different natures and its effects to final conclusions. We formulate a new approach to determining the range of reliability of the analytical continuation from imaginary chemical potential to its real values. We compute the ratios of the moments $\lambda_m$ in $N_f = 2$ lattice QCD and compare results with the values extracted from the RHIC experimental data.

In the next section we briefly explain our lattice simulations. In Section III we describe the procedure to compute the canonical partition functions $Z_n$. Section IV is devoted to our results for the physical observables and comparison with respective experimental results. Finally, in Section V we conclude.

II. LATTICE SETUP

For simulating the lattice QCD at the imaginary chemical potential, we employ the clover improved Wilson fermion action with two flavors and Iwasaki gauge action. The details of the simulation were reported in Ref. [10]. Our simulation corresponds to $m_\pi/m_\rho = 0.8$ ($m_\pi = 0.7$ GeV). In this report, we study two temperatures: $T/T_c = 1.35(7)$ ($\beta = 2.0$) corresponds to the deconfinement phase and $T/T_c = 0.93(5)$ ($\beta = 1.8$) - the confinement phase.

In the confinement (deconfinement) phase we make simulations at 27(37) different values of the baryon chemical potential $\mu_B$ in the interval $0 \leq \mu_B/T \leq \pi$. Additionally we make simulations at a few values of $\mu_B$ above $\pi$ to check the Roberge-Weiss periodicity. For each value of $\mu_B$ 1800 configurations separated by ten trajectories are used to evaluate the physical observables.

III. COMPUTATION OF $Z_n$

Using standard lattice QCD algorithms, we can evaluate the baryon number density $n_B$ directly for any value of the imaginary chemical potential:

$$\frac{n_B}{T^3} = iC \int DU e^{-S_G(\det \Delta(\mu_I))} \text{Tr} \left[ \Delta^{-1} \frac{\partial \Delta}{\partial \mu_I/T} \right],$$  

where $C = \frac{N_f N_s^3}{24 \pi^3}$. Note that the number density in imaginary chemical potential regions is pure imaginary.

On the other hand, the number density is connected with the canonical partition function, $Z_n$ as

$$n_B = \frac{\lambda_1}{V} = \frac{T}{V} \frac{\partial}{\partial \mu_B} \ln Z_{GC}(\mu_B, T)$$

$$= \frac{i}{(aN_c)^3} \frac{2}{\sum_{j=1}^{N_{max}} Z_n n \sin(n\theta_I)}$$  

where we used Eq. (4) and relation $Z_n = Z_{n,-}$. The direct way to extract the canonical partition functions $Z_n$ from the lattice data for $n_B$ is fit to the measured baryon number density to Eq. (8) with $Z_n$ as fitting parameters. We tried to fit it and realized that the fit goes quite unstable and some $Z_n$’s are negative. The difficulty of fitting comes from the drastic cancellations in both the numerator and denominator in Eq. (8).

More promising way is to construct the grand canonical partition function from $n_B$. Integrating number density over imaginary $\mu_I$, at fixed temperature $T$, we have

$$\frac{Z_{GC}(\theta_I)}{Z_{GC}(0)} = \exp \left( \int_0^{\theta_I} d(\bar{\theta}_I) i \text{Im}[n_B(\theta_I)] \right)$$

$$= \exp \left( -V \int_0^{\theta_I} dx n_{BI}(x) \right),$$  

where we use the fact that $n_B$ is pure imaginary and denote $n_{BI} = \text{Im} n_B$. We calculate $Z_n$ by inserting this $Z_{GC}$ into Eq. (8). Then one can construct $Z_{GC}$ as $Z_{GC} = \sum Z_n e^{\xi_n}$ at real $\mu_B$. This procedure provides a new method to study physics in the real chemical potential region via Monte Carlo simulations of the pure imaginary chemical potential [10,11].

There is no Ansatz until this point; therefore, Eq. (9) is exact and theoretically the calculation for any value of the chemical potential is possible. In practice, however, we must introduce some assumptions, and consequently, the reliable range of the real chemical potential values is restricted.

One way to evaluate the right hand side in Eq. (9) is to calculate the number density for many values of $\mu_I$ and complete the numerical integration. In order to obtain a reliable result, we need hundreds of different $\mu_I$ values, but this is computationally expensive task. In this letter we employ a simple approach - we fit the numerical data for $n_B$ and use the fit function in Eq. (8). Thus the idea is to fit the number density as a function of $\mu_I$ to
Ansatz Eq. (10) and (11) given below, to compute the partition function for imaginary $\mu_B$ from Eq. (9), then to compute $Z_n$ using Eq. (5). This idea is a continuation of another concept in Refs. [18, 20] - fit the data at imaginary $\mu_B$ and do analytical continuation to the real axis. The authors of Ref. [8] have recently reported a thorough analysis. In Refs. [18, 20], the authors pointed out that the number density for the imaginary chemical potential is well approximated by a Fourier series at $T < T_c$,

$$n_{BI}(\theta_1)/T^3 = \sum_{k=1}^{k_{max}} f_{3k} \sin(k\theta_1), \quad (10)$$

and by a polynomial series at $T > T_c$ [21],

$$n_{BI}(\theta_1)/T^3 = \sum_{k=1}^{k_{max}} a_{2k-1} \theta_1^{2k-1}. \quad (11)$$

In Refs. [16, 17] we confirmed these conclusions with higher precision. Therefore in the present study in computation of $Z_{GC}(\theta)/Z_{GC}(0)$, we use parameterizations Eqs. (10) and (11). We obtained the best fits for $k_{max} = 2$ with $f_3 = 0.0871(3)$ and $f_6 = -0.00032(27)$ ($\chi^2$/dof = 0.93) at $T/T_c = 0.93$, $a_1 = 1.5570(7)$, $a_3 = -0.3300(13)$ ($\chi^2$/dof = 0.67) at $T/T_c=1.35$ for our data $n_{BI}$. For careful error analysis we performed calculations for different $k_{max}$.

To estimate the statistical error, we apply a version of a bootstrap method: here one bootstrap sample consists of a set of standard bootstrap samples of the number density created for every value of $\mu_I$. On each bootstrap sample, we estimate $n_B$ with Eq. (10) ($T < T_c$) or Eq. (11) ($T > T_c$) (coefficients $f_{3k}$ or $a_{2k-1}$ are different on each sample), and calculate $Z_n$ according to Eq. (9) and (5). Then, using these $Z_n$ and Eq. (6) with number of terms restricted to $n_{max}$, we calculate observables.

It is important to note that the baryon number density fitted to Eqs. (10) or (11) can be analytically continued to the real chemical potential values - it was previously studied in Refs. [16, 18, 20].

Baryon number density can be fitted to different functions at imaginary chemical potential with good precision but when we make analytical continuation to the real chemical potential we obtain substantially different results for high enough $\mu_B$. There are no strict arguments about how to choose unique fitting function. For this reason range of reliable values of $\mu_B$ (where all good fitting functions predict same results) might be small. Consequently determination of the reliable range for analytic continuation is problematic. Another problem of this method is that, the phase transition may be missed because it implies breaking of analyticity.

On the other hand, the canonical approach provides us with useful information on the range of reliability at real real chemical from the physics. From relation $Z_n = \langle n|e^{-\hat{H}}|n \rangle$ it follows that $Z_n$ must be positive. If $Z_n$ become negative for some $n > n_{max}$ it means that respective Ansatz for the number density used for $Z_n$ calculation via Eq. (9) and (5) can not describe physics for these $n$. In the statistical analysis as described above, we used only positive $Z_n$. It is important to note that in each bootstrap sample $n_{max}$ can be different due to slightly different coefficients in Ansatz.

We then compute observables from Eq. (6) using $Z_n$ for $n \leq n_{max}$. Respective result for the number density coincides within numerical precision with that obtained via analytic continuation at small enough values of $\mu_B/T$. However, it starts to deviate at larger values of $\mu_B/T$. The value of $\mu_B/T$ where this deviation becomes substantial determines the range of reliability of the analytic continuation. We will illustrate this procedure in the next section.

![FIG. 1. Normalized $Z_n$ as a function of $n$ obtained by the integration method for different number of terms (sines) in Ansatz (Eq. (10)) - $k_{max}$. HPE stands for $Z_n$ calculated using Hopping Parameter Expansion, which are taken from Ref. [16]. Temperature $T/T_c = 0.93$ (Confinement).](image)

![FIG. 2. Same as Fig. 1 but for temperature $T/T_c = 1.35$ (Deconfinement) and polynomial Ansatz (Eq. (11)).](image)
In the Fig. 1 and 2 one can see $Z_n/Z_0$ calculated with
different number of terms $k_{\text{max}}$ in Eq. (10) and (11).
At $T/T_c = 0.93$ the error of two-term Ansatz is large
due to propagation of large relative error of $f_0$, i.e.,
noise from our statistics and discrepancy between $k_{\text{max}} = 1$
and $k_{\text{max}} = 2$ is small. At $T/T_c = 1.35$ the behavior for
varying $k_{\text{max}}$ is similar. For comparison we also present
$Z_n$ calculated with winding number expansion method
in hopping parameters expansion approximation (labeled
by HPE on figures) borrowed from Ref. 10. For polynomial
fits starting from some $n = n_{\text{max}}$ value the sign of
$Z_n$ starts to alternate while the absolute value changes
very slowly. Thus we conclude that polynomial series can
describe the data only for relatively small fixed $n_{\text{max}}$ or
$\mu_{\text{reliable}}$. For fits (10) with even $k_{\text{max}}$ similar thing hap-
pens: starting from some $n_{\text{max}}$ there appears alternation
of the sign of $Z_n$. We thus conclude that the Fourier fits
with even $k_{\text{max}}$ should be also avoided or used for the
range of $n$ values below respective $n_{\text{max}}$.

IV. PHYSICAL QUANTITIES

A. Baryon number density

With $Z_n$ calculated using Fourier Ansatz in the con-
finement phase and polynomial Ansatz in the deconfin-
ment phase with different $k_{\text{max}}$, we calculate the baryon
number density for the real baryon chemical potential
$\mu_B$ values via Eq. (9) with restricted number of terms to
$n_{\text{max}}$. The results are shown in Figs. 3 and 4. For large
$\mu_B/T$, the number density obtained via Eq. (9) goes to
plateau as a consequence of the finite number terms in
respective sums. This effect allows us to estimate re-
liability range of our calculation in real $\mu_B$. The po-

tion $\mu_{\text{reliable}}/T$ where baryon density goes to plateau
is determined by $n_{\text{max}}$: the bigger $n_{\text{max}}$ is, the bigger
$\mu_{\text{reliable}}/T$. On insets of Figures 4 and 3 we present data
with different $n_{\text{max}}$: results coincide up to $\mu_{\text{reliable}}/T$
where number density goes to constant. Therefore we
conclude that systematical error due to truncation in (4)
affects only on determination of $\mu_{\text{reliable}}/T$ and do not
change results for reliable range. We expect that increas-
ing of statistics will allow us to increase $n_{\text{max}}$.

From figures 1 and 3 it is clear that our data for baryon density
becomes unreliable after $\mu_{\text{reliable}}/T \sim 4 - 5$ at
$T/T_c = 0.93$ and $\mu_{\text{reliable}}/T \sim 2 - 2.5$ at $T/T_c = 1.35$.
For comparison we also presented the data for direct
analytical continuation ($k_{\text{max}} = 2$) and Taylor expansion
method (Taylor coefficients were borrowed form 22).

FIG. 3. The baryon number density for the real chemical
potential at $T/T_c = 0.93$ calculated using integration method
with different number of terms $k_{\text{max}}$ in Ansatz Eq. (10).
At insert the effect of finite number of $Z_n - n_{\text{max}}$ is shown for
$k_{\text{max}} = 2$. For comparison we also present direct analytical
continuation (for $k_{\text{max}} = 2$) and Taylor expansion method
with two coefficients $c_1$ and $c_2$ taken from 22.

FIG. 4. Same as Fig. 3 but for temperature $T/T_c = 1.35$ and
Ansatz Eq. (11).

FIG. 5. Baryon number density for RHIC data of different
energies $\sqrt{s_{NN}}$ (s in figure) in GeV together with our lattice
results for temperatures $T/T_c = 0.93$ and $T/T_c = 1.35$. 
The canonical partition functions $Z_n$ can be directly extracted from an experiment on heavy ions collision. Indeed, the multiplicity distributions $P_n$ measured in experiment have a sense of probability and consequently connected with $Z_n$: $P_n = Z_n \xi^n$. Accordingly to this argument in Ref. [23] $Z_n$ as well as fugacity were extracted from the RHIC experiments data. At that, authors compared extracted fugacity with different works on estimation of freeze-out parameters and got agreement within $5\%$. With $Z_n$ extracted from RHIC data [23], we construct the baryon number densities by Eq. (8) for each RHIC energy. See Fig. 5 where we show also our lattice results at $T/T_c = 0.93$ (black) and $1.35$ (red). We see, as the baryon number density calculated on the lattice at $T > T_c$ deviates from RHIC data, while in the confinement the experimental data can be consistent with the lattice calculation except $\sqrt{s_{NN}} = 11.5$. Estimated temperature at $\sqrt{s_{NN}} = 11.5$ in Ref. [24] is significantly below other energy data.

B. Moments of the baryon number density

One can construct $\lambda_2/\lambda_1$ and $\lambda_4/\lambda_2$ from these $Z_n$. In Figs. 6 and 7 we show these ratios as calculated by the integration method described above together with those extracted from the RHIC Star data.

In the relativistic heavy-ion collision experiments, $\lambda_2/\lambda_1$ and $\lambda_4/\lambda_2$ (kurtosis) are expected to be good indicators for detecting the QCD phase transition [2, 23]. We calculate these quantities and compare with experiments.

Note that $Z_n$ were constructed from the proton multiplicity data, not the baryon multiplicity. Therefore, the results should be considered as a proxy for the real baryon number moments. Nevertheless, in the confinement regions we see very good agreement for $\lambda_2/\lambda_1$ and $\lambda_4/\lambda_2$ between the lattice calculation and those estimated from RHIC data. It is important to point out that for high $\mu_B/T$ the ration $\lambda_2/\lambda_1$ goes from 1 to 0 as expected for phase transition. According to our study it does not indicate phase transition and position of this transition is shifted with varying of $n_{max}$. Therefore this transition just indicates us the position of $\mu_{reliable}$ for this observable. Because of the fact that for RHIC data we have only small $Z_n$ number, i.e., $n_{max}$ reliability range for it is much smaller, we estimate it as $\mu_{reliable}/T \sim 1.2 - 2.5$ depending on $\sqrt{s_{NN}}$.

Repeating the same procedure with varying $n_{max}$ the reliability range for $\lambda_2/\lambda_1$ can also be estimated. It is interesting that for this observable $\mu_{reliable}/T$ is much smaller than for baryon density of $\lambda_2/\lambda_1$. For all RHIC data (except $\sqrt{s_{NN}} = 11.5$) it is much smaller than our prediction and we estimate it as $\mu_{reliable}/T \sim 0.3 - 0.45$.

V. CONCLUDING REMARKS

In this letter, we study an approach for revealing the QCD phase structure using lattice QCD simulations. Prior to this study, it was believed that this was impossible because of the sign problem; only small density regions could be studied by extrapolating from the data at $\mu_B/T = 0$. However, all relevant information on the QCD phase at finite baryon density is contained in the imaginary chemical potential regions, $0 \leq \mu_I/T \leq \pi$. The question is how to map this information to the real chemical potential. Eq. (4) provides a possible solution, because $Z_n$ can be calculated in the imaginary chemical potential regions. Since numerical Monte Carlo simulations provide results with finite accuracy, we should find practical methods which work.

We fit the number density at the imaginary chemical potential using $Z_n$ as parameters and found that it does not work.

We parametrize the number density in the imaginary chemical potential with the Ansatz (the Fourier series in the confinement and polynomial series in the decon-
finement) and integrate them to get the grand partition function. The canonical partition function, $Z_n$, and other observables are then calculated from them.

This method produces $Z_n$ up to $n_{max}$ which is determined by used Ansatz and current statistics. However, this is not the first principle calculation because of introducing an assumption to the number density. Analyzing $n_{max}$ behavior we can estimate reliability of this assumption. On the other hand, better interpolation procedure (cubic spline for example) or numerical integration rather than any Ansatz release our data from assumptions. This study will be reported in future.

We studied how errors of calculations made at the imaginary chemical potential propagate into errors at the real one. We also found range of reliability of our results by imposing the condition that $Z_n$ have to be positive.

We then investigate whether we can estimate $\lambda_3/\lambda_1$ and $\lambda_3/\lambda_2$. The results are consistent with the values estimated from the RHIC experiments as shown in Figs. 8 and 7. This is very encouraging. More realistic simulations with the physical quark mass and small lattice spacing, may even predict the temperature of the experimental data.

When we map the information from pure imaginary to real chemical potential by the canonical method, the reliable regions for baryon density is $\mu_{\text{reliable}}/T \sim 4 - 5$ at $T/T_c = 0.93$ and $\mu_{\text{reliable}}/T \sim 2 - 2.5$ at $T/T_c = 0.93$. This limitation comes from the finite numbers of $Z_n$ as a consequence of polynomial (in the deconfinement phase) /Fourier (in the confinement phase) Ansatz. They can be increased by increasing of statistics.

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