A new way of determining the QCD equation of state at a finite chemical potential

Sabarnya Mitra\textsuperscript{1} and Prasad Hegde\textsuperscript{1}

\textsuperscript{1}Centre for High Energy Physics, Indian Institute of Science, Bangalore, India

Abstract

The Taylor expansion of thermodynamic observables at a finite baryon chemical potential $\mu_B$ is an oft-used method to circumvent the well-known sign problem. A reliable Taylor estimate demands sufficiently high-ordered calculations in chemical potential $\mu$ for a proper estimate of its radius of convergence. But, owing to the associated difficulty and limitations of precision in calculating these high-ordered Taylor coefficients, it becomes essential to look for various alternative expansion schemes which can mitigate the computational cost, besides providing trustworthy estimates of different thermodynamic observables. Resummation to all order in $\mu$ is one such promising alternative scheme. Recently, a way to resum the contribution of the first $N$ charge density correlation functions $D_1, \ldots, D_N$ to the Taylor series to all orders in $\mu_B$ was proposed in Phys. Rev. Lett. 128, 2, 022001 (2022). The resummation resembles the form of an exponential factor. Since the correlation functions $D_n$ are calculated stochastically using estimates from different random volume sources, the resummation formulation gets affected by the emergence of biased estimates. The effects from these estimates can become very drastic and can radically misdirect the calculations for large values of $N$ and $\mu$ and also for observables which are higher order $\mu$ derivatives of free energy, specially at lower temperatures. In this work, we present a cumulant expansion procedure that allows to investigate and regulate these biased estimates at different orders in $\mu$. We find that the unbiased estimates in the cumulant expansion can truly capture the genuine higher-order stochastic fluctuations of the higher order correlation functions, which got suppressed by the exponential resummation formulation. Finally, we discover an unbiased formalism of the exponential resummation, which when expanded in a series, can exactly reproduce the Taylor series up to a desired power in $\mu$. We are also able to regain the knowledge of reweighting factor and many other important properties of the partition function, which got entirely lost through the implementation of cumulant expansion scheme.

1 Introduction

The QCD Equation of State (EoS), illustrating the QCD Phase diagram is of significant importance in the parlance of QCD phase transitions and also in the study of heavy-ion collisions [1–4]. Primarily, the phase diagram elucidates the low temperature hadronic phase and the high temperature partonic or quark-gluon plasma (QGP) phase. In principle, the entire phase diagram can be completely explained from a comprehensive study of the gauge theory of QCD. But, in reality, it is still a conjecture from a practical standpoint, with many salient and robust features remaining to be established. Hence, for a proper unfazed conclusion, an unambiguous thermodynamic approach is adopted, which revolves around the important calculations of the estimates of various thermodynamic observables.

The system considered, resembles a grand canonical ensemble of quarks interacting via gluons, sufficiently described by a grand canonical partition function $Z(\mu, V, T)$. In principle, the partition function is given as a path integral over all the constituent particle (quark) and gauge field (gluon) configurations.
Unfortunately, this path integral formulation of \( Z \), yields an intractable, infinite-dimensional integral. Although lattice QCD averts this problem by rendering this integral to a solvable finite-dimensional one, the complex integral measure of \( Z \) at a finite \( \mu \) inhibits the implementation of Monte-Carlo importance sampling (MCIS). By virtue of the reweighting procedure [5–8], although the measure being weighted at zero \( \mu \) becomes real, the complex measure problem assumes the form of the notorious sign problem [9–11], getting manifested in the observable part of the integral. But on the positive side, reweighting enables the application of MCIS for the calculation of \( Z \) by making the integral measure semi positive definite.

The Taylor expansion of thermodynamic observables upto the first \( N \) coefficients [12, 13] as a function of \( \mu \) is one of the numerous methods [14–20] adopted to evade the sign problem. Owing to the slow rate of convergence and non-monotonic behaviour of the Taylor series for a wide range of temperatures, it is essential to calculate upto sufficiently high orders in \( \mu \), which invokes calculation of higher-order Taylor coefficients. This directs one towards resummation of Taylor series [21–26], which allows one to conduct an all-ordered calculation with the knowledge of a few Taylor coefficients. The exponential resummation [27] is one such resummation method which is instrumental in our work.

In this work, we present the mathematical form of Taylor expansion and exponential resummation. We then comprehensively discuss about the emergence of biased estimates in exponential resummation, which has the potential to become highly problematic in the regime of large values and higher orders of \( \mu \). We then come across the formulation of cumulant expansion [28–32], which allows an order-by-order analysis of biased estimates, but unfortunately at the cost of the reweighting factor and hence, the invaluable partition function itself. Finally, we present an unbiased formulation of exponential resummation, which reproduces the Taylor (QNS) expansion upto a given order of \( \mu \) [12, 13], apart from a newly defined reweighting factor and partition function altogether. Most significantly, this formalism paves a possible pathway towards achieving a fully unbiased all-ordered exponentially resummed formulation.

### 2 Setup of the simulation

In our work, we have used Highly Improved Staggered Quark (HISQ) action [33–35] for the fermions and tree-level improved Symanzik gauge action for the gauge fields. The work has been done using 2+1 flavor QCD with \( m_u = m_d = m_s/27 \), where \( m_u, m_d \) and \( m_s \) are the masses of up, down and strange quarks respectively. With a fixed lattice spacing and coupling parameter \( \beta \), the quark masses are tuned appropriately to their physical values, so that they produce physical pion and kaon masses, as directed by chiral perturbation theory (\( \chi \)PT). This therefore fixes the line of constant physics (LCP) for our work [12, 36, 37], which is governed by \( m(\beta) \). Also, the work has been performed on a lattice with temporal extent \( N_T = 8 \) and spatial extent \( N_\sigma = 32 \). We have collected gauge configurations for three temperatures at \( T = 135, 157 \) and 176 MeV, which in \( \beta \) scale, corresponds to \( \beta = 6.245, 6.390 \) and 6.500 respectively. These three temperatures were specifically chosen to establish the temperature or regime independence of our formalism, since 135 MeV resides in the hadronic regime, 176 MeV in the QGP phase with 157 MeV lying in the crossover region for the chosen values of the quark masses. Also the data for the traces are available for \( 135 \leq T \leq 176 \) MeV within the directory of the relevant data for our work. We have worked with 20K configurations for both baryon (\( \mu_B \)) and isospin (\( \mu_I \)) chemical potentials. Recent work is in progress to increase the statistics for \( \mu_B \) by increasing the number of gauge field configurations. Although we worked mostly upto \( D_4 \), all the eight derivatives \( D_1, D_2, \ldots, D_8 \) are calculated stochastically using \( O(500) \) random volume sources (RVS) per configuration. All these correlation functions \( D_n \) for \( n \leq N \) can be expressed as different linear combinations of traces [25, 38], involving products of fermion propagator \( M^{-1} \) and different ordered \( \mu \) derivatives of fermion matrix \( M \). The stochastic calculation arises mainly because the computation of \( M^{-1} \) cannot be performed exactly. A detailed description of the gauge ensembles and scale setting can be found in Ref. [13].
3 Taylor series and Exponential Resummation

The Taylor expansion of excess pressure $\Delta P/T^4 = P(\mu, T)/T^4 - P(0, T)/T^4$ and number density $N/T^3$, in terms of $\mu_B$ up to the first $N$ derivatives \[12, 13\] are given by

$$\frac{\Delta P_N^Q(T, \mu_B)}{T^4} = \frac{1}{VT^3} \ln \left[ \left( \frac{\mathcal{Z}(\mu)}{\mathcal{Z}(0)} \right) \right] = \sum_{n=1}^{N} \frac{X_{2n}}{(2n)!} \hat{\mu}_B^{2n}$$

$$\frac{\mathcal{N}_N^Q(T, \mu_B)}{T^3} = \frac{\partial}{\partial \hat{\mu}_B} \left[ \frac{\Delta P_N^E}{T^4} \right] = \sum_{n=1}^{N} \frac{X_{2n}}{(2n - 1)!} \hat{\mu}_B^{2n-1}$$

where $X_n$ are the $n$th order quark number susceptibilities (QNS) and $\hat{\mu}_B = \mu_B/T$. The CP symmetry of QCD \[25\] ensures that pressure and number density constitutes even and odd series in $\mu_B$ respectively. The exponentially resummed estimate of excess pressure is given by

$$\frac{\Delta P_N^R(T, \mu_B)}{T^4} = \frac{1}{VT^3} \ln \left( \text{Re} \left\{ \exp \left( \sum_{n=1}^{N} \overline{D}_n(T) \hat{\mu}_B^n \right) \right\} \right), \quad \overline{D}_n(T) = \frac{1}{N_R} \sum_{r=1}^{N_R} \hat{D}_n^{(r)}(T)$$

where $\hat{D}_n^{(r)}(T) = \frac{D_n^{(r)}(T)}{n!}$ and $D_n^{(r)}(T) = \frac{\partial^n}{\partial \hat{\mu}_B^n} \ln \left| \det M^{(r)}(T, \mu_B) \right|_{\mu_B=0}$

The corresponding resummed estimate of number density is given by

$$\frac{\mathcal{N}_N^R}{T^3} = \frac{\partial}{\partial \hat{\mu}_B} \left[ \frac{\Delta P_N^R(T, \mu_B)}{T^4} \right]$$

where the expression for resummed excess pressure is given in eqn. (2). Here the angular brackets $\langle \rangle$ represent gauge ensemble average and $D_n^{(r)}$ is the $r$th estimate of the derivative $D_n$. In continuum limit, these derivatives are the integrated $n$-point correlation functions of the product of the zeroth component of the four baryon current density $J_0$ at different spacetime points $x$, given by $D_n = \int d^4x_1 d^4x_2 \ldots d^4x_n J_0(x_1) J_0(x_2) \ldots J_0(x_n)$ \[27\]. The CP symmetry dictates that all $D_n$ are real for even $n$ and imaginary for odd $n$ along with the fact that the partition function is real, for which only the real part of the exponential is taken into account in the above eqn. (2). It is therefore evident that

$$\Delta P_N^R/T^4 = \Delta P_N^Q/T^4 + \sum_{n>N} \left\langle (\overline{D}_1)^{A_1} (\overline{D}_2)^{A_2} \ldots (\overline{D}_N)^{A_N} \right\rangle \hat{\mu}_B^n$$

$$\mathcal{N}_N^R/T^3 = \mathcal{N}_N^Q/T^3 + \sum_{n>N} \left\langle (\overline{D}_1)^{A_1} (\overline{D}_2)^{A_2} \ldots (\overline{D}_N)^{A_N} \right\rangle \hat{\mu}_B^{n-1} \cdot n$$

where every $k$-point correlation function $D_k$ satisfies $\sum_{k=1}^{N} k \cdot A_k = n$. The number density $\mathcal{N}/T^3$ also exhibits similar comparative behaviour between the two approaches. By virtue of CP symmetry, $n$ in eqn. (4), is even, ensuring that the higher-order contributions for excess pressure involve only even powers of and that for number density consists of only odd powers of $\hat{\mu}_B$. 3
Problem of Biased Estimates and Cumulant Expansion

4.1 Biased estimates

As shown in Fig.1 and also in [27], the resummed results differ appreciably from the QNS counterparts in the regime of higher values of isospin chemical potential $\mu_I$. This stark difference arises from the higher order contribution terms, as indicated in eqn. (4). More significantly, as given in eqn. (2), the different powers of these different derivative estimates, from quadratic power onwards give rise to biased estimates. This is because, some given random vector estimates are raised to higher powers than the others, thereby treating different estimates on different footing in the sample of estimates.

\[
(D_n)^m = \left[\frac{1}{N_R} \sum_{r=1}^{N_R} D_n^{(r)}\right]^m = \left[\frac{1}{N_R} \sum_{r_1=1}^{N_R} \sum_{r_m=1}^{N_R} D_n^{(r_1)} ... D_n^{(r_m)}\right] \\
\approx \text{Biased estimate} + \left(\frac{1}{N_R}\right)^m \sum_{r_1 \neq ... \neq r_m}^{N_R} D_n^{(r_1)} ... D_n^{(r_m)}
\] (5)

The effects of these notorious biased estimates can become very pronounced and hence drastic, specially in the regime of large values of isospin chemical potential $\mu_I$ and also for higher powers of $\mu_I$ and estimating observables which are higher order $\mu_I$ derivatives of free energy. This therefore motivates one to truncate the resummed series in terms of different powers of $\mu_I$ and analyse the biased estimates for different orders of $\mu_I$. 

Fig 1. Pressure (left) and number density (right) plots as function of $(\mu_I/T)^2$ at 135 MeV. The resummed and QNS results are shown in bands, whereas the cumulant results (biased and unbiased) are shown in the form of points.
4.2 Cumulant Expansion

The cumulant expansion of eqn. (2) upto \( M \) cumulants in \( \mu_I \) yield (barring the \( 1/VT^3 \) factor)

\[
\ln \langle e^{X_N} \rangle = \sum_{n=1}^{M} \frac{\kappa_n^N}{n!} + O(\kappa_{M+1}^N), \quad X_N = \sum_{n=1}^{N} D_{2n}(T) \hat{\mu}_I^{2n} \tag{6}
\]

We exploited the efficacy of cumulant expansion for \( \mu_I \), where there is no sign problem, because of the vanishing odd-ordered derivatives and also because of which, \( X_N \) in eqn. (6) is manifestly real and we can safely work with \( O(10K) \) gauge configurations. We worked with only the first four cumulants (\( M = 4 \)) and computed biased and unbiased cumulants, where the biased cumulants \( \kappa^N_{b,n} \) are given by

\[
\begin{align*}
\kappa^N_{b,1} &= \langle X_N \rangle \\
\kappa^N_{b,2} &= \langle X_N^2 \rangle - \langle X_N \rangle^2 \\
\kappa^N_{b,3} &= \langle X_N^3 \rangle - 3 \langle X_N^2 \rangle \langle X_N \rangle + 2 \langle X_N \rangle^3 \\
\kappa^N_{b,4} &= \langle X_N^4 \rangle - 4 \langle X_N^3 \rangle \langle X_N \rangle + 12 \langle X_N^2 \rangle \langle X_N \rangle^2 - 6 \langle X_N \rangle^4 - 3 \langle X_N^2 \rangle^2
\end{align*} \tag{7}
\]

For unbiased cumulants \( \kappa^N_{u,n} \), we replace \( X_N^N \) with \( U_n[X_N] \) for each \( n \), in the cumulants of eqn. (7). Here \( U_n[X_N] \) is the unbiased \( n \)th power of \( X_N \), where \( X_N = \sum_{n=1}^{N} \overline{D}_n \hat{\mu}^n_B \) and unbiased \( n \)th power of \( D_m \) is given by

\[
U_n[D_m] = \frac{n!}{\prod_{k=0}^{n-1}(N_R - k)!} \sum_{r_1 \neq \ldots \neq r_n}^{N_R} D^{(r_1)}_m \ldots D^{(r_n)}_m \tag{8}
\]

Note that \( U_1[D_m] = m! \overline{D}_m \) \( \forall \) \( m \) and hence, we have \( U_n[X_N] = X_N \) \( \forall \) \( N \).

The biased \((B)\) and unbiased \((UB)\) excess pressure and number density, in terms of different cumulants are therefore given by

\[
\begin{align*}
\frac{\Delta P^{C(B)}_{N,M}}{T^4} &= \frac{1}{VT^3} \sum_{n=1}^{M} \kappa^N_{b,n} \frac{N^C_{N,M}}{n!} \frac{\partial}{\partial \hat{\mu}_B} \left[ \frac{\Delta P^{C(B)}_{N,M}}{T^4} \right] \\
\frac{\Delta P^{C(UB)}_{N,M}}{T^4} &= \frac{1}{VT^3} \sum_{n=1}^{M} \kappa^N_{u,n} \frac{N^C_{N,M}}{n!} \frac{\partial}{\partial \hat{\mu}_B} \left[ \frac{\Delta P^{C(UB)}_{N,M}}{T^4} \right]
\end{align*} \tag{9,10}
\]

As shown in the plots, the biased and unbiased results of pressure and number density as given by eqns. (9) and (10) are in good agreement with the resummed and QNS results of similar orders respectively. The unbiased cumulants managed to capture more higher-order fluctuations, which got suppressed by the exponential behaviour of the resummed series. The unbiased cumulant expansion results as in eqn. (10) hence, demonstrated that the difference between the resummed and QNS results is attributable to the difference between biased and unbiased estimates.

But, while incorporating unbiasedness at different orders, the truncation of the resummed series led to the loss of the reweighting factor and partition function altogether. This inspired the idea of a newly defined exponential resummation scheme which would, in principle reproduce QNS upto the desired order in \( \mu \). In addition, a numerically different partition function with an associated new reweighting factor is obtained, thereby re-enabling the essential calculations of phasefactor and roots of partition function.
5 Unbiased Exponential Resummation

Motivated by the isospin results, we have implemented this new formalism of an unbiased exponential resummation using baryon chemical potential $\mu_B$. Unlike $\mu_I$, the odd-ordered derivatives are non-vanishing and imaginary for $\mu_B$ and hence, it is necessary to extract the real part following eqn. (2) to obtain the expression of the partition function $Z_N$. In this formalism, all mathematical manipulations are done at the level of individual RVS present within every gauge configuration constituting the gauge ensemble. We have worked in two bases, which are stated as follows:

5.1 Chemical potential basis

In $\mu$ basis, with this new formalism, we define the unbiased pressure from a newly defined partition function following the usual prescription of the exponential resummation as follows:

$$\Delta P_{ub}^N(\mu) = \frac{1}{VT^3} \ln Z_{ub}^N(\mu), \quad Z_{ub}^N(\mu) = \left\langle \text{Re} \left[ \exp \left( A_N(\mu) \right) \right] \right\rangle,$$

$$A_N(\mu) = \sum_{n=1}^{N} \mu^n \frac{C_n}{n!}$$

where the $C_n$ for $1 \leq n \leq 4$ are given as follows:

$$C_1 = D_1,$$

$$C_2 = D_2 + \left( D_1^2 - D_1^2 \right),$$

$$C_3 = D_3 + 3 \left( D_2 D_1 - D_2 D_1 \right) + \left( D_1^3 - 3 D_1^2 D_1 + 2 D_1^3 \right),$$

$$C_4 = D_4 + 3 \left( D_2^2 - D_2^2 \right) + 4 \left( D_3 D_1 - D_3 D_1 \right) + 6 \left( D_2 D_1^2 - D_2 D_1^2 \right)$$

$$- 12 \left( D_2 D_1 D_1 - D_2 D_1^2 \right) + \left( D_1^4 - 4 D_1^3 D_1 + 12 D_1^2 D_1 + 6 D_1^4 - 3 (D_1^2)^2 \right)$$

Here, the powers of different $D_n$ are the unbiased powers of the respective different ordered derivatives, calculated as per eqn. (8). The analysis from this basis is important in the sense, that the degree of the unbiasedness in $\mu$ is exactly identical with the degree of the polynomial $A(\mu)$ as given in eqn. (11).

5.2 Cumulant basis

In cumulant basis, a new variable $W$ is defined, where $W_N = \sum_{n=1}^{N} \frac{\mu^n}{n!} D_n$, we have

$$\Delta P_{ub}^M(W_N) = \frac{1}{VT^3} \ln Z_{ub}^M(W_N), \quad Z_{ub}^M(W_N) = \left\langle \text{Re} \left[ \exp \left( Y_M(W_N) \right) \right] \right\rangle,$$

$$Y_M(W_N) = \sum_{n=1}^{M} \frac{L_n(W_N)}{n!}$$

which would reproduce exactly the first $M$ cumulants in unbiased cumulant expansion of excess pressure as given by unbiased version of eqn. (10). The different unbiased powers of derivatives are calculated as before, as given in eqn. (8). The $L_n(W)$ of eqn. (13) upto $M = 4$ for $1 \leq n \leq 4$ are as follows:
\[ L_1(W) = \langle W \rangle \]
\[ L_2(W) = \left[ \langle W^2 \rangle - \langle W \rangle^2 \right] \]
\[ L_3(W) = \left[ \langle W^3 \rangle - 3 \langle W^2 \rangle \langle W \rangle + 2 \langle W \rangle^3 \right] \]
\[ L_4(W) = \left[ \langle W^4 \rangle - 4 \langle W^3 \rangle \langle W \rangle + 12 \langle W^2 \rangle \langle W \rangle^2 - 6 \langle W \rangle^4 - 3 \langle W^2 \rangle^2 \right] \]

(14)

6 Results: Comparison between Biased and Unbiased formalism

The cumulant basis provides substantially more number of terms than \( \mu \) basis, specially for higher order of derivatives and higher order cumulants taken into account. Although we argue that \( \mu \) basis is useful for its manifest simplicity and first-principle understanding, the essence of cumulant basis lies in the fact that more higher-order contribution terms are considered. Different results demonstrate that it agrees well with the one order higher QNS results, as we expect from a resummation method, fortifying its efficacy and establishing at the same time, its faster convergence rate as well as the signature of a genuine series expansion, where the higher order contributions get reduced progressively. The results in unbiased resummation are carried out therefore primarily, in cumulant basis.

As mentioned before, the new formalism allows us to recalculate phasefactor and different thermodynamic observables. The 2\textsuperscript{nd} and 4\textsuperscript{th} ordered unbiased pressure results are in better agreement with the 4\textsuperscript{th} ordered QNS results than the old biased counterparts and the difference is stark and highly pronounced.
for 135 MeV. Surely, one can argue for higher statistics reducing the gauge noise, allowing the comparison for higher values of $\mu_B/T$. Also, one can even vouch to increase the number of RVS from 500 to even more, per gauge configuration, which is fine except that it will come at the cost of huge computational time and storage space, which are the two main concerns in computations.

However, despite all such arguments, the pressure plots demonstrate that even with a meagre 20K configurations with $O(500)$ random vectors per configuration, the new formalism attains excellent agreement with QNS over the old one, thereby saving profound computational time and storage space. The imaginary part of the argument in the exponential function constitutes the phase-angle, the cosine of which forms the phasefactor in the biased and unbiased cases. The phasefactor plots show that the biased and unbiased results do not vary very much, besides showing order-by-order agreement. This possibly indicates that the difference between pressure and phasefactor plots at 135 MeV is predominantly arising from phase quenched reweighting factor.

7 Conclusions

We have introduced a cumulant expansion which allows us to introspect the biased estimates and substitute them with unbiased counterparts order-by-order, in terms of $\mu_I$. The unbiased cumulant expansion, although truncated, managed to capture the higher-order fluctuations which the old exponential resummation could not efficiently serve to perform. But this comes at the cost of resummation and the significant partition function itself. We then, therefore introduce a new exponential resummation formalism, which unlike the old resummation [27], exudes an excellent agreement with the QNS results even using 20K configurations for $\mu_B$, with $O(500)$ random vectors per configuration. We also have managed to retrieve the partition function and hence, the complete thermodynamics altogether. More significantly, this partially unbiased exponential resummation gives an all-ordered unbiased exponential resummation reproducing the exact all-ordered QNS in the limit of an infinite cumulant expansion series.

The unbiased exponential resummed approach, outlined here is a new way of extending the QCD EoS. Nevertheless, the possible connections between the approach presented here and various other proposals in the literature [22, 39–41] still remain to be explored and therefore serve to be the promising ingredients for numerous future works.

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