New formalism for unbiased exponential resummation of Taylor series in Lattice QCD at a finite baryon chemical potential

Sabarna Mitra$^1$ and Prasad Hegde$^1$

$^1$Centre for High Energy Physics, Indian Institute of Science, Bangalore 560012, India
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The exponential resummation of Taylor series in lattice QCD at a finite temperature $T$ and baryon chemical potential $\mu_B$ is a significant improvement over the Taylor series and provides reliably better estimates of the finite density QCD equation of state. However, due to the stochastic estimation of the fermion propagator, this resummation formula involves stochastic bias which if not treated, can lead to wrong results. In this paper, we introduce a new formalism of unbiased exponential resummation that eliminates stochastic bias up to a desired order in $\mu_B$, by including unbiased corrections and modifying the argument of the exponential function. We implement this formalism and present consequent results for excess pressure, number density and average phasefactor at $T = 135$ MeV, where this bias is significant. We demonstrate that despite having significant bias, this formalism not only eliminates bias to a given order in $\mu_B$ but also produces better results manifesting higher order Taylor contributions.

**Introduction** – A comprehensive exploration of the Quantum Chromodynamics (QCD) phase diagram[1–7] and a detailed study of the QCD Equation of state [8–11] is paramount not only for understanding the dynamics of strong interactions, but also for constructing the physics of the early universe [12–14]. For this a reliable non-perturbative approach is required, one of which is formulating QCD on a lattice discretised spacetime [15–20] at finite $T$, $\mu_B = 0$. Unfortunately for $\mu_B \neq 0$, the fermion sign problem restricts lattice QCD computations leading to an eventual breakdown of calculations for finite density QCD [21–23]. Among the several methods that have been proposed to avoid the sign problem [24–27, 29–34], the method of Taylor expansions [26–28] has yielded reliable results for the QCD Equation of State at moderately large chemical potentials [35]. However, owing to the difficulty of computing the higher order Taylor coefficients, this method requires modifications for its applicability at larger values of $\mu_B/T$ [36–38].

In this regard, Padé resummation [36, 37] of the QCD Taylor series has been successfully applied [35, 39] to the resummation of the QCD Taylor series. Besides Padé resummation, another important resummation is the exponential resummation [40] where the contributions of the $n$th baryon correlation function $D_n$ [41], resummed to all orders, is of the form exp ($\mu_B^n D_n / n!$). This offers to provide an all-orders resummation estimate of the QCD partition function.

Despite its obvious advantages, the exponential resummation results get affected by the presence of stochastic bias, which is not the case for the usual Taylor series. One way to avoid this bias, without resorting to Taylor series is to replace exponential resummation by cumulant expansion to some finite order in $\mu_B$ [42]. In this method, although the bias gets eliminated to a given order in $\mu_B$, the all-orders resummation and reweighting factor along with the phasefactor gets lost, following which we lose sight of the analytic structure of the QCD partition function and QCD thermodynamics at finite baryon density.

In this paper, we introduce a new formalism, which by retaining the exponential form of resummation along with a valid reweighting factor and phase factor, produces unbiased estimates of $D_n$ to a given order in $\mu_B$ and replicates Taylor series to that order exactly. We illustrate these novel features at 135 MeV which being the lowest temperature in our working data, exhibits largest magnitude of stochastic bias in usual resummation calculations. We demonstrate that this new formalism at 135 MeV not only removes this bias to a desired order in $\mu_B$, it also captures higher order Taylor contributions for both imaginary and real values of $\mu_B$ up to the breakdown value of $\mu_B$. We also show that the ensemble-averaged phasefactor for unbiased calculations drop to zero more quickly than the biased counterparts.

**Biased estimates** – We consider a system of 2+1 flavor QCD with physical values of $u, d, s$ quark masses. The partition function $Z$ at a finite $T$, $\mu_B$ is given as

$$Z(T,\mu_B) = \int DU e^{-S_G[T,U]} \text{det} \mathcal{M}(T,\mu_B,U)$$

with fermion matrix $\mathcal{M}$, gauge field configuration $U$ and gauge action $S_G[U]$. We suppress the gauge dependence of $\mathcal{M}$ from here on and work in relativistic units with unit Boltzmann constant. In thermodynamic limit for a system of volume $V$ at a temperature $T$, we know the following relations for dimensionless pressure ($P$) and number density ($N$):

$$\frac{P(T,\mu_B)}{T^4} = \frac{1}{VT^3} \ln Z(T,\mu_B),$$
$$\frac{N(T,\mu_B)}{T^3} = \frac{\partial}{\partial(\mu_B/T)} \left[ \frac{P(T,\mu_B)}{T^4} \right]$$

The excess pressure at $\mu_B$ is defined as $\Delta P(T,\mu_B) =$
$P(T, \mu_B) - P(T, 0)$. The Taylor expansion of excess pressure to $O(\mu_B^N)$ is given as follows:

$$\frac{\Delta P_N^T}{T^4} = \sum_{n=1}^{N/2} c_{2n} \left( \frac{\mu_B}{T} \right)^{2n}$$

(3)

The Taylor coefficients $c_{2n}$ can be obtained as follows:

$$c_{2n} = \left. \frac{1}{(2n)!} \frac{\partial^{2n} \Delta P_N^T}{\partial (\mu_B)^{2n}} \right|_{\mu_B=0}$$

(4)

where $\mu_B \equiv \mu_B/T$. The $n^{th}$ order Taylor coefficient $c_n$ can be expressed as linear combinations of terms having the form $\langle D_1^n D_2^n \ldots D_N^n \rangle^{(unb)}$ satisfying $\sum_{r=1}^{N} \beta \cdot P_{\beta} = n$ and where $D_n$ are temperature dependent $n$-point baryon correlation functions given as

$$D_n(T) = \left. \frac{\partial^n \ln \det \mathcal{M}(T, \mu_B)}{\partial (\mu_B)^{n}} \right|_{\mu_B=0}$$

(5)

We suppress the temperature dependence of $D_n$ from here on. At finite $T$, the exponential resummation of excess pressure to $O(\mu_B^N)$ yields:

$$\Delta P_N^R \langle T^4 \rangle = \frac{1}{VT^3} \ln \left[ \text{Re} \left( \left\langle \exp \left( \sum_{n=1}^{N} \hat{\mu}_B^n D_n n^! \right) \right\rangle \right) \right]$$

(6)

The resummed and Taylor number densities are obtained using Eq. (2). As the $D_n$ in Eq. (6) are purely real( imaginary) for even(odd) $n$, the exponential factor is complex even for real $\mu_B$ and can be written as $R_N(T, \mu_B) e^{i \Theta_N(T, \mu_B)}$ where

$$R_N(T, \mu_B) = \exp \left( \text{Re} \left( \sum_{n=1}^{N} \hat{\mu}_B^n D_n n^! \right) \right)$$

$$\Theta_N(T, \mu_B) = \text{Im} \left( \sum_{n=1}^{N} \hat{\mu}_B^n D_n n^! \right)$$

(7)

The imaginary part of the exponential in Eq. (6) vanishes when averaged over all gauge configurations, since $Z$ must be real-valued for real $\mu_B$ for physical $\Delta P$. Anticipating this, we have written $\text{Re} \langle \cdot \rangle$ in Eq. (6) and hence the partition function $Z$ is constructed using the real part of the ensemble average. Similarly, the imaginary part of $e^{i \Theta_N(T, \mu_B)}$ also vanishes upon averaging, due to which we have denoted the phasefactor as $\cos \Theta$.

These $D_n$ are obtained from linear combinations of traces involving $\mathcal{M}^{-1}$, using the familiar identity $\det e^{\mathcal{M}} = e^{\text{Tr} \mathcal{M}}$ for non-singular matrix $\mathcal{M}$. Since $\mathcal{M}^{-1}$ is analytically inexact, hence these $D_n$ are estimated using finite number of random volume sources $N_{rv}$, inside every gauge configuration of the working gauge ensemble. So, on a lattice with $N_s$ spatial sites and $N_T$ temporal sites with lattice spacing $a$, Eq. (6) modifies to

$$\Delta P_N^R \langle T^4 \rangle = \left( \frac{N_T}{N_s} \right)^3 \ln \left[ \text{Re} \left( \left\langle \exp \left( \sum_{n=1}^{N} \hat{\mu}_B^n D_n n^! \right) \right\rangle \right) \right]$$

(8)

where $D_n$ is given by

$$D_n = \frac{1}{N_{rv}} \sum_{r=1}^{N_{rv}} D_n^{(r)}$$

(9)

In the above Eq. (8), we use the usual relations on lattice, $T = (aN_T)^{-1}$ and $V = (aN_s)^3$. $D_n^{(r)}$ represents the estimate of $D_n$ in $r^{th}$ random volume source. Using the series expansion of exponential function in Eq. (8) and Eq. (9), one finds biased estimates [42] of $D_n$. The unbiased exponential resummation formalism eliminates these biased estimates to the desired order in $\mu_B$.

The unbiased Exponential Resummation – In this formalism, the idea is to modify the argument of the exponential and change it accordingly so that after the series expansion of “exp” and “ln” functions (see Eq. (8)), $\Delta P_N^R \langle T^4 \rangle$ becomes identical to Taylor excess pressure $\Delta P_N^T/T^4$ (see Eq. (3)), to $O(\mu_B^N)$. We deduce this formalism for $\mu_B$ in two bases as follows:

a) Chemical potential basis – In chemical potential basis for $\mu_B$, we define the unbiased excess pressure from a newly defined partition function, following the usual prescription of the exponential resummation as follows:

$$\Delta P_N^{R(unb)}(T, \mu_B) = \frac{1}{VT^3} \ln Z_N^{R(unb)}(T, \mu_B),$$

$$Z_N^{R(unb)}(T, \mu_B) = \text{Re} \left\langle \exp \left( A_N(T, \mu_B) \right) \right\rangle,$$

$$A_N(T, \mu_B) = \sum_{n=1}^{N} \hat{\mu}_B^n \frac{C_n}{n^!}$$

(10)

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

ensemble generated at $\mu_B = 0$ for a given $T$.
\[ C_1 = D_1, \]
\[ C_2 = D_2 + \left[ (D_1)^2 - (D_1)^2 \right], \]
\[ C_3 = D_3 + 3 \left[ D_2 D_1 - (D_2)(D_1) \right] + \left[ (D_1)^3 - 3 (D_1)^2 (D_1) + 2 (D_1)^3 \right], \]
\[ C_4 = D_4 + 3 \left[ (D_2)^2 - (D_2)^2 \right] + 4 \left[ D_3 D_1 - (D_3)(D_1) \right] + 6 \left[ (D_2)(D_1)^2 - (D_2)(D_1)^2 \right] - 3 [(D_1)^2]^2 \]
\[ - 12 \left[ (D_2 D_1)(D_1) - (D_2)(D_1)^2 \right] + \left[ (D_1)^4 - 4 (D_1)^3 (D_1) + 12 (D_1)^2 (D_1)^2 - 6 (D_1)^4 \right] \]  

Here in Eqn. (11), \((D_n)^p\) indicates average of \(p^{th}\) unbiased power of \(D_n\) over all the \(N_{rv}\) random volume sources contained within the gauge configuration. The necessary formulae are enlisted in Ref.[42]. The quartic degree of the polynomial \(A_N(\mu)\) indicates appearance of unbiased estimates up to \(\mathcal{O}(\mu_B^4)\). The average phasefactor to \(\mathcal{O}(\mu_B^N)\) in this basis is denoted by \(\cos \Theta_R^{(\text{unb})}(\mu)\), where

\[ \Theta_R^{(\text{unb})}(\mu) = \text{Im} \left[ \sum_{n=1}^{N} \tilde{\mu}_B^n C_n(T) \right] \]  

**b) Cumulant basis** – In cumulant basis for \(\mu_B\), a new variable \(X_N\) is defined, where \(X_N = X_N(T, \mu_B) = \sum_{n=1}^{N} \tilde{\mu}_B^n D_n/n!\) with \(\tilde{\mu}_B = \mu_B/T\). The unbiased excess pressure along with a newly defined partition function in this basis is defined as follows:

\[ \frac{\Delta P_{R,(\text{unb})}}{T^4}(T, \mu_B) = \frac{1}{V T^3} \ln Z_{R,(\text{unb})}(T, \mu_B), \]
\[ Z_{R,(\text{unb})}(T, \mu_B) = \text{Re} \left[ \exp \left( W_M [X_N(T, \mu_B)] \right) \right], \]
\[ W_M [X_N(T, \mu_B)] = \sum_{m=1}^{M} \mathcal{L}_m(X_N)/m! \]  

which reproduce exactly the first \(M\) cumulants in unbiased cumulant expansion of excess pressure as highlighted in Ref.[42]. The \(\mathcal{L}_m(X_N)\) upto \(M = 4\) are:

\[ \mathcal{L}_1(X_N) = \overline{X_N} \]
\[ \mathcal{L}_2(X_N) = \overline{(X_N)^2} \]
\[ \mathcal{L}_3(X_N) = \overline{(X_N)^3} - 3 \overline{(X_N)^2} \overline{(X_N)} + 2 \overline{(X_N)^3} \]
\[ \mathcal{L}_4(X_N) = \overline{(X_N)^4} - 4 \overline{(X_N)^3} \overline{(X_N)} - 3 \overline{(X_N)^2}^2 \]
\[ + 12 \overline{(X_N)^2} \overline{(X_N)^2} - 6 \overline{(X_N)^4} \]  

The average phasefactor to \(\mathcal{O}(\mu_B^N)\) with \(M\) cumulants in this basis is denoted by \(\cos \Theta_R^{(\text{unb})}(\mu)\), where

\[ \Theta_R^{(\text{unb})}(\mu) = \text{Im} \left[ W_M [X_N(T, \mu_B)] \right] \]  

An explicit proof which shows how Eqsns. (11) and (14) remove bias up to \(\mathcal{O}(\mu_B^3)\) is presented in a related longer paper [43]. All the above calculations can be performed for determining number density \(N_{N,M}^{(\text{unb})}/T^3\), \(N_{N,M}^{(\text{unb})}/T^3\) in respective cumulant and chemical potential bases following the usual scheme as given in Eq. (2). So are the further higher order derivatives of \(\Delta P/T^4\). Inductively, one finds that for \(N \rightarrow \infty\) in Eq. (10) and for \(N, M \rightarrow \infty\) for Eq. (13), the unbiased exponential resummation formalism produces the exact infinite Taylor series of \(\Delta P/T^4\) i.e. \(N \rightarrow \infty\) limit in Eq. (3).

**Results** – As an illustration of the advantages of the formalism presented above, we apply exponential resummation to the HotQCD collaboration’s Taylor expansion data for \(N_r = 8\) at \(T = 135\) MeV\(^2\) [44]. On the same sample of 100,000 configurations, we calculated \(\Delta P(T, \mu_B)/T^4\) and \(N(T, \mu_B)/T^3\) using:

\[ \text{Figure 1. Results for } 2^{nd} \text{ order excess pressure } \Delta P_2(T, \mu_B)/T^4 \text{ at } T = 135 \text{ MeV. The bands illustrate the Taylor series results for the respective orders. The unbiased resummation calculations in cumulant and chemical potential bases are shown using black and green points respectively. The red and blue points illustrate the old biased resummed results for 500 and 2000 random vectors respectively.} \]

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2 Similar results for \(T = 157\) and 176 MeV have been presented in a related longer paper [49].
Since resummation is supposed to capture the contribution of higher orders, we calculated the Taylor expansion to one higher order than either resummation. We shall compare the $N = 2$ resummation results to $N = 2$ and $N = 4$ Taylor expansion results, and similarly the $N = 4$ resummation results to $N = 4$ and $N = 6$ Taylor expansion results.

The HotQCD data consist of 500 stochastic estimates of $D_1, \ldots, D_8$ for each gauge configuration. For $D_1$, the data also contain an additional independent set of 2000 stochastic estimates. The operator $D_1$ appears with the highest power among all derivatives at any order $N$. As a result, controlling the fluctuations in $D_1$ contributes significantly to decreasing the overall statistical error. While performing the biased resummation, we obtained results both with and without the additional 2000 random vectors. However, the unbiased resummation results which we will present here were obtained without using the additional 2000 estimates. By doing so, we achieved a comparable improvement in the results. This was without using additional random vectors and with all derivatives treated on an equal footing.

We note that the chiral crossover temperature is equal to $T_{pc} = 156.5(1.5)$ MeV [45]. This implies that our working temperature $T = 135$ MeV lies in the hadronic part of the QCD phase diagram. For $N_F = 8$, the lattice spacing $a$, as determined from $T = (a N_F)^{-1}$, is quite large and in fact, the gauge coupling $\beta$ lies in the strong coupling region for this temperature. Since the off-diagonal elements of $\mathcal{M}$ comprise $\exp(\mu\tau)$, this makes the condition number of matrix $\mathcal{M}$ maximum at 135 MeV. Due to this large condition number, huge fluctuations are observed among different random volume estimates of $\mathcal{M}^{-1}$ and $D_n$, which eventually leads to significant differences between the $p^{th}$ biased and unbiased powers of $D_n$. These differences increase more with increasing $n$ and $p$, and also at lower temperatures. This happens because in biased powers, a particular random volume estimate out of the entire sample of estimates is raised to higher powers whereas for unbiased powers, all the stochastically generated random volume estimates in the sample are considered independently with each on equal footing. Hence, unbiased powers prove to be a better statistical tool and measure for computational calculations, especially when working with a stochastic sample of random volume estimates storing values of $D_n$ for every single gauge field configuration.

In Fig. 1, we compare our results for the excess pressure, obtained using second order resummation, with the results from second and fourth order Taylor expansions. The red points were calculated using Eq. (8) using only the initial 500 stochastic estimates for $D_1$. The blue points were also calculated using Eq. (8), but using 2000 stochastic estimates for $D_1$. We see that the increased number of estimates for $D_1$ has a significant effect on the results. The former results are close to zero while the latter results are clearly non-zero and much closer to the Taylor expansion results. These results are thus indicative of the presence of stochastic bias, which needs to be accounted for before the genuine higher order contributions can be identified.

We note that the fourth order Taylor expansion results (orange band) only slightly correct the second order results (purple band) over the entire range of chemical potentials, namely $-1.5 \leq (\mu_B/T)^2 \leq 1.5$. The Taylor expansion results thus suggest that higher order contributions to the second order results should be small. When we turn to the unbiased resummation results, we find that both the cumulant and chemical potential basis results (green and black points) are in very good agreement with the fourth order Taylor expansion results over the entire range. Although both the bases eliminate stochastic bias completely to $O(\mu_B^2)$, the cumulant basis yields more number of unbiased estimates to higher orders in $\mu_B$ in
addition to chemical potential basis. Despite this, the appreciable agreement between the results of the two bases indicate that bias at higher orders is negligible. Note that these results were obtained using only 500 stochastic estimates for \(D_1\). This also suggests that although only being unbiased to second order, our formalism still produces a result that is close to the fully unbiased result. Similar results are also obtained for the fourth order excess pressure as well as for the second and fourth order net baryon density (Fig. 2).

It is well known that lattice calculations at a finite real \(\mu_B\) suffer from a sign problem. The sign problem also limits the maximum value of \(\mu_B\) to which extrapolations, such as reweighting or Taylor series expansion, can be trusted. In the case of Taylor series, this limiting value is the radius of convergence \(\rho = |\mu_B^0|\), where \(\mu_B^0\) is the closest singularity to the origin in the complex \(\mu_B\) plane. However, as the formula \(\rho = \lim_{n \to \infty} \sqrt{c_{2n}/c_{2n+2}}\) shows, a knowledge of the first several Taylor coefficients is necessary in order to obtain a reasonable estimate. By contrast, exponential resummation yields a phase factor even at second order. As \(\mu_B\) is increased from zero, the expectation value of the phase factor decreases from unity, becoming zero at some value \(\mu_B = \mu_B^0\). From Fig. 1 and Fig. 2, we see that this happens around \(\mu_B^0 \sim 1.5\). Beyond this value, the resummation calculation breaks down. The approach to breakdown manifests as a sudden increase in the error due to the rapid oscillations of the phase factor. For \(\mu_B > \mu_B^0\), the average value of the exponential is close to zero and hence the pressure (Eq. (6)) cannot be determined.

In Fig. 3, we present our results for the expectation value of the real part of the average phase factor \(\langle \cos \Theta(T, \mu_B) \rangle\), calculated using both the biased and unbiased formalisms. Within each individual formalism, we find no difference between our second order and fourth order results. However, we see a clear difference between the results of the biased and unbiased formalisms, with the latter decreasing more rapidly and going to zero at a smaller value of \(\mu_B^0\) than the former. However, among the unbiased formalisms we do not see much difference between the chemical potential and cumulant bases. The unbiased phase factor vanishes for \(\mu_B^0 \sim 1.2\), corresponding to the value \(\mu_B^0 \sim 1.5\) at which, as we have seen, our pressure and number density calculations break down. By contrast, the phase factor in the biased formalism goes to zero only around \(\mu_B \sim 1.5\). Thus we see that it is necessary to first take stochastic bias into account to also obtain a reliable estimate of the maximum value \(\mu_B^0\) for which the resummation, and hence the Taylor series calculations, can be trusted.

\(\text{Discussions and Outlook} -\) We have introduced a new formalism of unbiased exponential resummation which eliminates stochastic bias in the resummation while computing thermodynamic observables as a function of \(\mu_B\) to a desired order in \(\mu_B\). We provided evidence for the same through results for the excess pressure and the net baryon density at \(T = 135\) MeV, calculated for both real as well as imaginary \(\mu_B\). This is performed for both 2nd and 4th order calculations in \(\mu_B\), where the stochastic bias gets eliminated upto \(O(\mu_B^2)\) and \(O(\mu_B^4)\) respectively. Most importantly, the unbiased calculations, carried out with only \(O(500)\) random volume sources for each derivative, yielded better results than biased resummation with 2000 random vectors for the derivative \(D_1\). At the temperature presented here viz. \(T = 135\) MeV, the biased resummation differed from the Taylor expansion results by nearly an order of magnitude. The new formalism on the other hand, remains efficient even at this temperature, where the effects of stochastic bias are highly pronounced.

The ability of exponential resummation to capture higher order Taylor series in imaginary \(\mu_B\) makes it promising for calculations where one deduces real finite \(\mu_B\) equation of state by analytically continuing from simulations performed at imaginary \(\mu_B\). On repeating this calculation to higher orders in \(\mu_B\) or to more number of cumulants, one finds that this formalism approaches an exponential resummation which is unbiased completely to all orders in \(\mu_B\). This becomes equivalent to the infinite Taylor series in \(\mu_B\). Importantly, this argument as well as the aforementioned formalism holds true for \(\mu_S\) and \(\mu_I\) also, where \(D_n\) will subsequently represent strangeness and isospin \(n\)-point correlation functions. This therefore leads us to conclude that this formalism is equally valid for any other arbitrary chemical potential apart from \(\mu_B\).

\(^3\) The expectation value \(\langle \sin \Theta(T, \mu_B) \rangle\) of the imaginary part of the phase factor is identically equal to zero since \(Z(T, \mu_B)\) is real for real \(\mu_B\).
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