A New Way Of Resumming Qcd At A Finite Chemical Potential

Sabarnya Mitra

Centre for High Energy Physics, Indian Institute of Science, Bangalore

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Outline of the talk

- Motivation and Introduction
- Taylor Series Expansion
- Exponential Resummation
- Bias in Exponential Resummation
- Cumulant Expansion
- An unbiased exponential formalism
- Conclusions and Outlook



Motivation and Introduction



- In principle, QCD can explain the above phase diagram completely
- Unfortunately, in reality, it still remains to be a **conjectured** one
- A grand canonical prescription is followed, forming the ensemble along with a grand canonical partition function $\mathcal{Z}(\mu, V, T)$
- The formulation is done by remaining in a **non-perturbative** regime
- The estimates of excess pressure and number density are considered here
- Initially, the setup of calculation is being briefly discussed



Computational Setup

- The present work has made use of $2{+}1{-}{\rm flavor}$ HISQ ensembles for three temperatures at T = 135 , 157 and 176 MeV
- The quark masses are tuned to their respective physical values.
- The calculations have been performed on a $32^3 \cdot 8$ lattice for all three T's.
- Within every gauge configuration, the scaled n-point correlation functions \tilde{D}_n are calculated stochastically using random volume sources of $\mathcal{O}(500)$
- We have considered only upto 4 point correlation functions $(1 \le n \le 4)$
- The work is done with an ensemble of 20 K gauge field configurations
- The computations are mostly done with μ_B
- A few also done with μ_I as the sign problem is evaded



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Taylor Series (TS) Expansion

• In form of a Taylor series (TS) in μ_B , the excess pressure is given by

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

$$QNS: \mathcal{X}_{2n} = \frac{\partial^{2n}}{\partial(\mu_B/T)^{2n}} \left[\frac{\Delta P}{T^4}\right]\Big|_{\mu_B=0}$$
(1)

• The number density in a Taylor form, is given by

$$\frac{\mathcal{N}}{T^3} = \frac{\partial}{\partial(\mu_B/T)} \left[\frac{\Delta P}{T^4}\right] = \sum_{n=1}^N \frac{\mathcal{X}_{2n}}{(2n-1)!} \left(\frac{\mu_B}{T}\right)^{2n-1} \tag{2}$$

- There is a slow convergence rate and non-monotonic behaviour
- It is therefore essential to calculate TS to sufficiently high orders in μ_B
- Calculation of high-order TC are very tedious, computationally expensive
- Is there any possible way around ?
- The immediate solution is an **all-ordered resummation** maybe



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A brief on Resummation methods

- Primarily, two methods of resummation are briefly enlightened here
- The Padé resummation provides important Padé approximants
- They are useful in approximating the behaviour of a function near a given value of the argument
- Which is done by a rational function of an order, equal to that of the TS being approximated
- They may work in certain domains where Taylor approximations fail to converge

►►► For a more detailed explanation, please refer to the TALKS ON "Isentropic equation of state in (2+1) flavor QCD" by

Jishnu Goswami

"Multi-point Padé for the study of phase transitions" by Francesco Di Renzo

- The present work is focused on a second method of resummation
- Which is the **exponential resummation** method



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Exponential Resummation (ER)

• The resummed estimate to all orders in μ_B for $D_n(1 \le n \le N)$ is given by

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

where $\langle \cdot \rangle$ is the expectation value over all possible gauge field configurations in an ensemble **generated at** $\mu_B = 0$ with N_R random vectors per configuration [S. Mondal, S. Mukherjee, P. Hegde, Phys. Rev. Lett **128**, 022001 (2022)]

• D_n are *n*-point correlation functions which are real for even *n*, imaginary for odd *n*, given by

$$\tilde{D}_n = \frac{D_n}{n!} = \frac{1}{n!} \left. \frac{\partial^n}{\partial \hat{\mu}_B^n} \ln \det M\left(T, \hat{\mu}_B\right) \right|_{\mu_B = 0} \qquad (\hat{\mu}_B \equiv \mu_B/T).$$
(4)

• Hence, $\Delta P_N^R(T, \hat{\mu}_B) = \Delta P_N^E(T, \hat{\mu}_B) + \sum_{n>N}^{\infty} \langle \overline{D}_1^i \overline{D}_2^j \dots \overline{D}_N^k \rangle \ \hat{\mu}_B^n$, where $1 \cdot i + 2 \cdot j + \dots + N \cdot k = n$.



A major but hidden problem: Bias

- The highly useful ER suffers from the emergence of biased estimates
- That is purely by virtue of the way the series is constructed
- In principle, they manifest when the derivative estimate from at least one random vector, is raised at least to quadratic integral powers

$$(\overline{D}_n)^m = \left[\frac{1}{N_R}\sum_{r=1}^{N_R} D_n^{(r)}\right]^m = \left[\left(\frac{1}{N_R}\right)^m \sum_{r_1=1}^{N_R} \dots \sum_{r_m=1}^{N_R} D_n^{(r_1)} \dots D_n^{(r_m)}\right]$$

$$\approx \text{Biased estimate} + \sum_{r_1 \neq \dots \neq r_m}^{N_R} \dots \sum_{r_m \neq m}^{N_R} D_n^{(r_1)} \dots D_n^{(r_m)}$$
(5)

• These effects can prove to be very drastic in the long run involving

- Large values of μ
- Higher orders of μ in series expansion
- Higher order μ derivatives of free energy
- It is therefore high time we try to identify and minimise their emergence and subsequent effects in calculations





Plots of pressure (left) and number density (right) [S. Mondal, S. Mukherjee, P. Hegde, Phys. Rev. Lett **128**, 022001 (2022)]

- The different **unbiased powers** of D_n are used for constructing TC in QNS
- There is **no such scope** to introduce unbiased powers within the given formulation of ER with **transcendental functions** being present
- The above pressure and number density plots clearly indicate the significant difference between the two approaches for large orders and values of μ
- This is clearly attributable to biased and unbiased estimates
- Hence, one is motivated to truncate the ER series in such a manner so that the truncated series reproduces QNS upto $\mathcal{O}(\mu_B^N)$



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Cumulant Expansion (CE): Formalism

• Considering $X = \sum_{n=1}^{N} \frac{\mu^n}{n!} \overline{D}_n$, the cumulant expansion (CE) of ER series in eqn. (3) yields (barring the $1/VT^3$ factor)

$$\ln\left\langle e^X\right\rangle = \sum_{n=1}^M \frac{\kappa_n}{n!} + \mathcal{O}(\kappa_{M+1}) \tag{6}$$

where κ_n is the *n*th cumulant, N represents the highest derivative order and M is the total number of cumulants

- $|\Delta P^C_{N,M}|/T^4$ and $\mathcal{N}^C_{N,M}/T^3$ are calculated with M=4 with N=2,4
- The first 4 cumulants in X are represented as follows

$$\kappa_{1} = \langle X \rangle,$$

$$\kappa_{2} = \langle X^{2} \rangle - \langle X \rangle^{2},$$

$$\kappa_{3} = \langle X^{3} \rangle - 3 \langle X^{2} \rangle \langle X \rangle + 2 \langle X \rangle^{3}$$

$$\kappa_{4} = \langle X^{4} \rangle - 4 \langle X^{3} \rangle \langle X \rangle + 12 \langle X^{2} \rangle \langle X \rangle^{2} - 6 \langle X \rangle^{4} - 3 \langle X^{2} \rangle^{2}$$
(7)

[S. Mitra, P. Hegde, and C. Schmidt, (2022), arXiv:2205.08517]

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• The higher-order fluctuations are truly captured by the unbiased cumulant estimates, which used to get suppressed by ER

- A good agreement is observed between
 - biased cumulant and ER (Δ and red bands)
 - unbiased cumulant and QNS (∇ and **blue bands**)



Cumulant Expansion: Debacle

- Despite the **all-important** introduction of unbiasedness in the calculations, the cumulant expansion does **deprive** us of some things which are as follows
 - 1. The reweighting factor
 - 2. The partition function ${\mathcal Z}$
 - 3. The phasefactor
 - 4. The singularities of partition function \mathcal{Z} in the complex $\hat{\mu}_B$ plane
- The obvious search is therefore to **retrieve back** everything lost, but **preserving unbiasedness**
- Is that achievable ?



A possible unbiased ER formula: idea

- The idea is to search for an unbiased counterpart of ER which would reproduce unbiased powers exactly up to $\mathcal{O}(\mu^N)$
- In this new formalism, all mathematical manipulations are done with the the sample of random volume sources available within every gauge configuration constituting the configuration ensemble
- In μ basis, the new formalism resembles the following shape

$$P_{ub}^{\mu} = \frac{1}{VT^3} \ln \mathcal{Z}_{ub}^{\mu}, \quad \mathcal{Z}_{ub}^{\mu} = \left\langle e^{A(\mu)} \right\rangle, \quad A(\mu) = \sum_{n=1}^{N} \mu^n \frac{\mathcal{C}_n}{n!}$$
(8)

where the C_n (different μ coefficients) for n = 1, 2, 3, 4 are given as follows:

Different μ coefficients

$$\begin{split} \mathcal{C}_{1} &= \overline{D_{1}}, \\ \mathcal{C}_{2} &= \overline{D_{2}} + \left(\overline{D_{1}^{2}} - (\overline{D_{1}})^{2}\right), \\ \mathcal{C}_{3} &= \overline{D_{3}} + 3\left(\overline{D_{2}D_{1}} - (\overline{D_{2}})(\overline{D_{1}})\right) + \left(\overline{D_{1}^{3}} - 3(\overline{D_{1}^{2}})(\overline{D_{1}}) + 2(\overline{D_{1}})^{3}\right), \\ \mathcal{C}_{4} &= \overline{D_{4}} + 3\left(\overline{D_{2}^{2}} - (\overline{D_{2}})^{2}\right) + 4\left(\overline{D_{3}D_{1}} - (\overline{D_{3}})(\overline{D_{1}})\right) + 6\left(\overline{D_{2}D_{1}^{2}} - (\overline{D_{2}})(\overline{D_{1}^{2}})\right) \\ &- 12\left((\overline{D_{2}D_{1}})(\overline{D_{1}}) - (\overline{D_{2}})(\overline{D_{1}})^{2}\right) + \\ &\left(\overline{D_{1}^{4}} - 4(\overline{D_{1}^{3}})(\overline{D_{1}}) + 12(\overline{D_{1}^{2}})(\overline{D_{1}})^{2} - 6(\overline{D_{1}})^{4} - 3(\overline{D_{1}^{2}})^{2}\right), \end{split}$$

• The simplicity of this basis is highlighted by the fact that the degree of the unbiased QNS expansion, being reproduced by this method is exactly identical to the degree of the polynomial $A(\mu)$, being exponentiated

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Cumulant basis: The second one

• In **cumulant basis**, a new variable W is defined, where

$$W = \sum_{n=1}^{N} \frac{\mu^n}{n!} D_n \neq X$$
, we have

$$P_{ub}^W = \frac{1}{VT^3} \ln \mathcal{Z}_{ub}^W, \quad \mathcal{Z}_{ub}^W = \left\langle e^{Y(W)} \right\rangle, \quad Y(W) = \sum_{n=1}^M \frac{\mathcal{L}_n(W)}{n!} \tag{9}$$

• which would reproduce exactly the first M cumulants in UCE

$$\ln\left\langle e^{Y}\right\rangle = \sum_{n=1}^{M} \frac{\kappa_{n}^{ub}}{n!} + \mathcal{O}(\kappa_{M+1}) \tag{10}$$

- N cumulants in cumulant basis is equivalent to having unbiased powers to $\mathcal{O}(\mu^{\mathbf{N}})$ for $\mu = \mu_{(B,Q,S)}$ and $\mathcal{O}(\mu^{\mathbf{2N}})$ for $\mu = \mu_I$
- The first four \mathcal{L}_n in eqn. (9) and κ_n^{ub} in eqn. (10) are explained as follows

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$$\mathcal{L}_{1} = (\overline{W})$$

$$\mathcal{L}_{2} = \left[\left(\overline{W^{2}} \right) - \left(\overline{W} \right)^{2} \right]$$

$$\mathcal{L}_{3} = \left[\left(\overline{W^{3}} \right) - 3 \left(\overline{W^{2}} \right) \left(\overline{W} \right) + 2 \left(\overline{W} \right)^{3} \right]$$

$$\mathcal{L}_{4} = \left[\left(\overline{W^{4}} \right) - 4 \left(\overline{W^{3}} \right) \left(\overline{W} \right) + 12 \left(\overline{W^{2}} \right) \left(\overline{W} \right)^{2}$$

$$- 6 \left(\overline{W} \right)^{4} - 3 \left(\overline{W^{2}} \right)^{2} \right]$$
(11)

- The κ^{ub}_n are unbiased cumulants resembling eqn. (7) with following transformation: Xⁿ ⇒ U_n[X] for n = 1, 2, 3, 4
- $U_n[X]$ is the unbiased *n*th power of X, $(X = \sum_{n=1}^{N} \frac{\mu^n}{n!} \overline{D}_n)$ given by

$$U_n[D_m] = \frac{n!}{\prod_{k=0}^{n-1} (N_R - k)!} \sum_{r_1 \neq \dots \neq r_n}^{N_R} \dots \sum_{r_1 \neq \dots \neq r_n}^{N_R} D_m^{(r_1)} \dots D_m^{(r_n)}$$

• A faster rate of convergence with more higher-order terms ensure that cumulant basis is the preferred basis to work with



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Pressure (left) and phasefactor (right) plots for T = 135 and 157 MeV



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Roots of \mathcal{Z}



Roots of \mathcal{Z}_2 and \mathcal{Z}_4 in complex μ_B plane at 135 MeV

- The unbiased formalism **ensures** a newly defined partition function $\mathcal Z$
- It is therefore **possible** to search for roots of \mathcal{Z} in the complex $\hat{\mu}_B$ plane
- The green outline represents a naive lower bound of the roots appearing in the complex $\hat{\mu}_B$ plane



Conclusions and Future Outlook

- A cumulant expansion has been established which duly serves as a bridge between a strict Taylor expansion (QNS) and old exponential resummation
- It has been possible to regulate the degree of unbiasedness at the level of individual cumulants and also at different powers of μ
- The unbiased (partially, in principle) exponential resummation, is guaranteed to provide exact unbiased results upto $\mathcal{O}(\mu^N)$
- Along with a newly defined reweighting factor and \mathcal{Z} , it has been possible to re-obtain phasefactor and roots of \mathcal{Z} in the complex μ_B plane
- Most significantly, it gives an **all-ordered unbiased exponentially** resummed series in the limit of a truly infinite cumulant series

In future, look for signs of **QCD critical point** by including **higher-order** derivatives



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BACKUP SLIDES



Plots of results from cumulant and μ bases



Pressure and number density plots in cumulant and μ bases for N = 2,4

- Cumulant basis provides **extra** higher order contribution terms over μ basis
- Fortunately, within the set of extra terms, we have terms and counter terms possibly
- Which nullifies the individual fluctuations among one another
- Faster convergence in cumulant basis over μ basis
- Making agreement with QNS, so good
- Hallmark of a genuine series expansion, where successive higher order contributions are less than the leading order



Phasefactor in cumulant and μ bases



Phasefactor plot at T = 135 MeV (cumulant and μ bases)

- Now, **can** calculate phasefactor
- Quite similar results for phasefactor from both the bases
- Plummeting to zero almost at the same value of μ_B/T



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Comparison between cumulant and μ bases

- The work on unbiased formalism is primarily done in the cumulant basis, as it provides a faster rate of convergence and a genuine series expansion as compared to μ basis
- The difference due to bias proved to be very acute and qualitatively radical at least in the case of 135 MeV results while working with $\hat{\mu}_B$
- The formalism obviate the bias to some extent, managing to agree along QNS results with negligible higher-order contributions

