A New Way To Determine Lattice QCD Equation Of State At A Finite Chemical Potential

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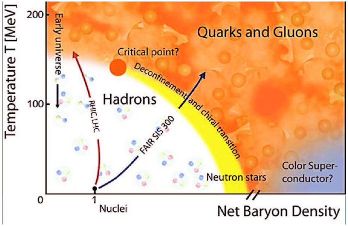
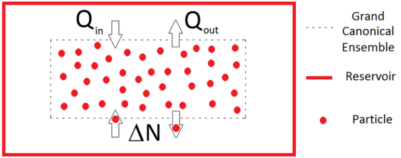
Motivation and Introduction



- The QCD phase diagram still remains to be **conclusively conjectured**
- Still in quest of conclusive evidences like a possible phase transition, **QCD critical point**, phases like **color superconductivity**, quarkyonic phases, extreme QCD (**neutron stars**)
- To answer, QCD **Equation of state** (EoS) is **crucial** to know
- Adopt a **thermodynamic** approach
- Observe the behaviour of thermodynamic observables with changing μ by remaining in a **non-perturbative** regime

Partition function and sign problem



- The ensemble : a **grand canonical ensemble** of quarks (u, d, s) in **thermal equilibrium** with a **reservoir** at temperature T
- Partition function $\mathcal{Z}(\mu, V, T) = \int \mathcal{D}\overline{\Psi}\, \mathcal{D}\Psi\, \mathcal{D}U\ \exp\left(iS_{QCD}[\overline{\Psi}, \Psi, U, \mu, V, T]\right) \rightarrow$ $\mathcal{Z}(\mu, T) \sim \int \mathcal{D}U\ e^{-S_g[U,T]}\ [\det\ \mathcal{M}(\mu, T, U)]$, with $\mathcal{M} \rightarrow$ fermion matrix
- **Complex** $\det \mathcal{M}(\mu)$ **inhibits** Monte-Carlo importance sampling
- With **reweighting** measure at $\boldsymbol{\mu = 0}$, we get **real** measure but observable becomes **complex** and **sign problem** comes due to phaseangle $\boldsymbol{\theta(\mu)}$: $\frac{\det \mathcal{M}(\mu)}{\det \mathcal{M}(0)} = \left|\frac{\det \mathcal{M}(\mu)}{\det \mathcal{M}(0)}\right| e^{i\theta(\mu)}$
- **Decreasing** $\langle \cos\theta \rangle$ with **increasing** μ, breakdown near $\boldsymbol{\langle \cos\theta \rangle \approx 0}$
- One way-around is **Taylor expansion** around $\mu = 0$

Taylor Expansion: Use of Random volume sources

- With $\hat{\mu} \equiv \mu/T$, the Taylor expansion of **excess pressure** $\Delta P = P(\mu) - P(0)$ and **number density** $\mathcal{N}$ to $\mathcal{O}(\mu^{\boldsymbol{N}})$ is given as

$$\frac{\Delta P}{T^4} = \sum_{n=1}^{N/2} C_{2n}\ \hat{\mu}^{2n}, \quad C_{2n} = \frac{1}{(2n)!}\frac{\partial^{2n}}{\partial \hat{\mu}^{2n}}\left[\frac{\Delta P}{T^4}\right]\Bigg|_{\mu=0} \tag{1}$$

$$\frac{\mathcal{N}}{T^3} = \frac{\partial}{\partial \hat{\mu}}\left[\frac{\Delta P}{T^4}\right] = \sum_{n=1}^{N/2} 2n\ C_{2n}\ \hat{\mu}^{2n-1} \tag{2}$$

- **CP symmetry** of QCD $\rightarrow$ eqn.(1) **even** and eqn.(2) **odd** in μ
- To calculate Nth order Taylor coefficient, we need to evaluate terms such as $\left\langle \boldsymbol{D}_1^{P_1} \boldsymbol{D}_2^{P_2} \cdots \boldsymbol{D}_N^{P_N} \right\rangle$, where $\mathcal{M}$ is fermion matrix and

$$\boldsymbol{D}_n = \frac{D_n}{n!} = \frac{1}{n!}\frac{\partial^n}{\partial \hat{\mu}^n} \ln\det \mathcal{M}\left(T, \hat{\mu}\right)\Bigg|_{\mu=0} \text{where } \sum_{\boldsymbol{k}=1}^{\boldsymbol{N}} \boldsymbol{k} \cdot \boldsymbol{P_k} = \boldsymbol{N} \tag{3}$$

- **Slow** convergence and **non-monotonic** behaviour of Taylor series for different N and T $\rightarrow$ **need** to do tedious calculations of higher order C_n $\rightarrow$ **motivates** exponential resummation of **lower** order Taylor series

Exponential Resummation

- The exponential resummed estimate of dimensionless excess pressure $\Delta P_N^R(T,\mu)/T^4$ to all orders in μ for $D_n (1 \leq n \leq N)$ is given by [S. Mondal, S. Mukherjee, P. Hegde, Phys. Rev. Lett **128**, 022001 (2022)]

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

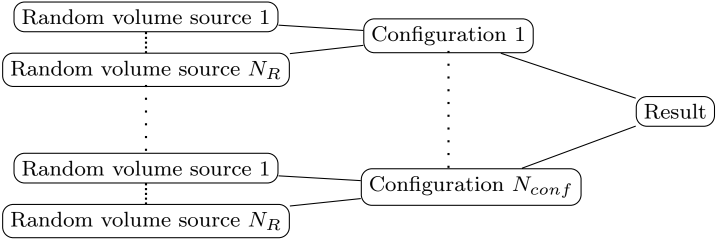
$$\frac{\mathcal{N}_N^R(T,\mu)}{T^3} = \frac{\partial}{\partial(\mu/T)}\left[\frac{\Delta P_N^R}{T^4}\right] \tag{5}$$

- **CP symmetry** : $\mathcal{Z}$ must be **real**, implying that **every** configuration estimate of $\mathcal{Z}$ must be real and so, extract the **real** part of the exponential.
- D_1 and D_2 can be expressed as follows:

$$D_1 = \mathrm{tr}\left[\mathcal{M}^{-1}\frac{\partial \mathcal{M}}{\partial \mu}\right], \; D_2 = \mathrm{tr}\left[\mathcal{M}^{-1}\frac{\partial^2 \mathcal{M}}{\partial \mu^2}\right] - \mathrm{tr}\left[\mathcal{M}^{-1}\frac{\partial \mathcal{M}}{\partial \mu}\mathcal{M}^{-1}\frac{\partial \mathcal{M}}{\partial \mu}\right]$$

- $\mathcal{M}^{-1}$ **cannot be evaluated exactly**, for which we need to therefore **estimate** D_n using N_R random volume sources for every configuration

Scheme of the structure



Stochastic Estimate of Trace

- The D_n in eqn.(4) are replaced with $\bar{D}_n$ (estimates of D_n) as follows

$$\bar{D}_n = \frac{1}{N_R} \sum_{r=1}^{N_R} D_n^{(r)}$$

- These $\bar{D}_n$ lead to **biased estimates** in exponential resummation

$$\left(\overline{D}_n\right)^m = \left[\frac{1}{N_R} \sum_{r=1}^{N_R} D_n^{(r)}\right]^m = \left[\left(\frac{1}{N_R}\right)^m \sum_{r_1=1}^{N_R} \dots \sum_{r_m=1}^{N_R} D_n^{(r_1)} \dots D_n^{(r_m)}\right]$$
$$\approx \text{Biased estimate} + \sum_{\boldsymbol{r_1 \neq \dots \neq r_m = 1}}^{N_R} \dots \sum^{N_R} D_n^{(r_1)} \dots D_n^{(r_m)} \quad (6)$$

- These biased estimates are **replaced** with **unbiased** estimates order-by-order through **cumulant expansion** of exponential resummed series [S. Mitra, P. Hegde, C. Schmidt, Phys Rev D.**106.034504**, arXiv:**2205.08517**]
- But, we **lose** partition function due to truncation of the series
- This motivates us towards **unbiased exponential resummation** to achieve unbiased thermodynamics

Two bases in brief

In $\boldsymbol{\mu}$ **basis**, we have

$$P^{\mu}_{ub,N} = \frac{1}{VT^3}\,\ln\,\mathcal{Z}^{\mu}_{ub,N}, \qquad \mathcal{Z}^{\mu,N}_{ub} = \left\langle e^{A_N(\mu)}\right\rangle, \qquad A_N(\mu) = \sum_{n=1}^{\boldsymbol{N}} \mu^n \frac{\mathcal{C}_n}{n!} \tag{7}$$

For $\boldsymbol{N = 4}$, this reproduces Taylor series upto $\mathcal{O}(\mu_{\boldsymbol{B}}^{\boldsymbol{4}})$ and $\mathcal{O}(\mu_{\boldsymbol{I}}^{\boldsymbol{8}})$

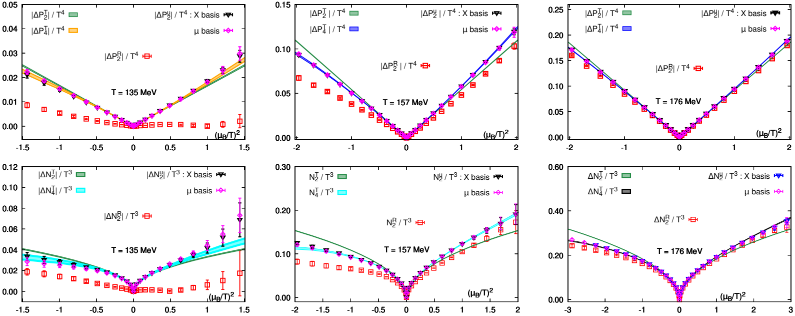
In **cumulant** or $\boldsymbol{X}$ basis, we define a new variable $X_N = \sum_{n=1}^{N} \frac{\mu^n}{n!} D_n$

$$P^{X,M}_{ub,N} = \frac{1}{VT^3}\,\ln\,\mathcal{Z}^{X,M}_{ub,N}, \quad \mathcal{Z}^{X,M}_{ub,N} = \left\langle e^{Y^M_N(X)}\right\rangle, \quad Y^M_N(X) = \sum_{n=1}^{\boldsymbol{M}} \frac{\mathcal{L}_n(X_N)}{n!} \tag{8}$$

Reproduces **exactly** first M cumulants of unbiased cumulant expansion

Captures **more higher-order contributions** over $\boldsymbol{\mu}$ **basis**

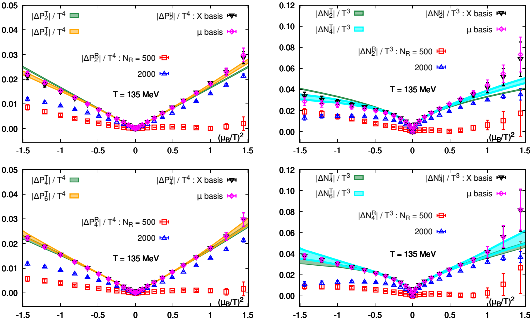
Results for three temperatures



$\Delta P_2/T^4$ (top row) and $\mathcal{N}_2/T^3$ (bottom row) plots in $(\mu_B/T)^2$ for 135 (left column), 157 (middle column) and 176 (right column) MeV

- We have used **$\mathcal{O}(500)$** volume sources per configuration for **both** biased and unbiased exponential resummed results
- Captures **higher-order** Taylor series even for lowest $\boldsymbol{T = 135}$ MeV,
- Also, **rapid** convergence → good agreement from lowest $N = 2$.

2000 random vectors for D_1

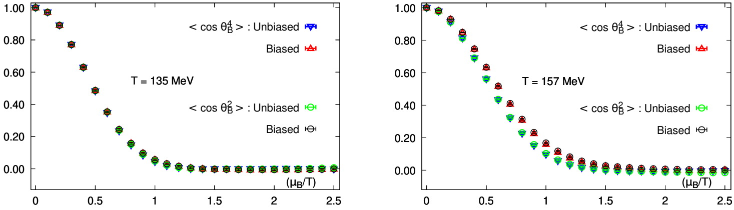


$\Delta P_{2,4}/T^4$ (left) and $\mathcal{N}_{2,4}/T^3$ (right) plots in both bases for $T = 135$ MeV

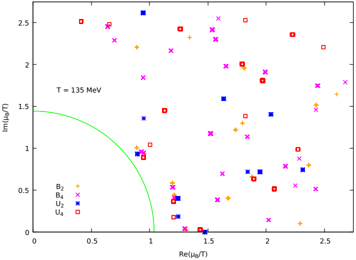
[S. Mitra, P. Hegde, arXiv:**2209.11937**]

- For **Biased** resummed results, we have used **2000** random volume sources for $\boldsymbol{D_1}$ and **500** random volume sources for **other** $\boldsymbol{D_n}$. For **unbiased** results, we have used **500** random volume sources for **all** $\boldsymbol{D_n}$
- **Higher order** Taylor series captured with **just** $\mathcal{O}(500)$ volume sources, **saving** appreciable **computational time** and **data storage space**

Phasefactor



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



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

Computational Setup

For all the above calculations, we have used the following data:

- **Physical** quark mass values for u, d, s quarks, where $\boldsymbol{m_u = m_d = m_s/27}$. This sets the crossover $\boldsymbol{T \approx 157}$ MeV at $\boldsymbol{\mu_B = 0}$
- Chosen $T =$ **135**, **157**, **176** MeV, characterizing **hadronic**, **crossover**, **quark gluon plasma** phases respectively.
- Temperatures are chosen so that $\left(\boldsymbol{T_{hadron}} + \boldsymbol{T_{plasma}}\right)/2 \approx \boldsymbol{T_{crossover}}$
- Considered lattice with $\boldsymbol{N_\sigma = 32}$ spatial sites and $\boldsymbol{N_\tau = 8}$ temporal sites
- Fermion action used is a $\boldsymbol{2+1}$ flavored **HISQ (Heavily Improved Staggered Quarks)** action
- For $\boldsymbol{\mu_I}$, we have used gauge ensemble having $\boldsymbol{20K}$ configurations and $\boldsymbol{100K}$ configurations for $\boldsymbol{\mu_B}$
- Because, there **is** a sign problem for $\boldsymbol{\mu_B}$. **No** sign problem for $\boldsymbol{\mu_I}$

Summary and Conclusions

- **Cumulant expansion** allows to **control** stochastic **bias**
- The idea of an **unbiased** exponential resummation
- Works efficiently for **all three** temperatures, including the problematic, yet important **low** T regime
- Highly effective in **saving** computational **time** and storage **space**
- Although not complete, but still to some finite order in μ
- Obtain an **unbiased** estimate of partition function $\boldsymbol{\mathcal{Z}}$ (**reweighting factor**)
- Get back knowledge of **phasefactor** and **roots** of $\mathcal{Z}$ in complex μ plane $\rightarrow$ **unbiased thermodynamics**
- **Inductively**, therefore going towards exponential resummation unbiased to **all orders** in μ, in the limit of an **all-ordered** argument.
- And this is **exactly identical** to the true **infinite Taylor series** of thermodynamic observables

THANK YOU SO MUCH

FOR YOUR PATIENCE AND ATTENTION !!!

μ basis

In $\boldsymbol{\mu}$ **basis**, we have

$$P_{ub}^{\mu,N} = \frac{1}{VT^3} \ \ln \ \mathcal{Z}_{ub}^{\mu,N}, \qquad \mathcal{Z}_{ub}^{\mu,N} = \left\langle e^{A_N(\mu)} \right\rangle, \qquad A_N(\mu) = \sum_{n=1}^{\boldsymbol{N}} \mu^n \frac{\mathcal{C}_n}{n!} \tag{9}$$

For $\boldsymbol{N = 4}$, we have (unbiased contributions upto $\mathcal{O}(\mu_{\boldsymbol{B}}^{\mathbf{4}})$ and $\mathcal{O}(\mu_{\boldsymbol{I}}^{\mathbf{8}})$)

$$\mathcal{C}_1 = \overline{D_1},$$

$$\mathcal{C}_2 = \overline{D_2} + \left(\overline{D_1^2} - (\overline{D_1})^2\right)$$

$$\mathcal{C}_3 = \overline{D_3} + 3\left(\overline{D_2 D_1} - (\overline{D_2})\,(\overline{D_1})\right) + \left(\overline{D_1^3} - 3\,(\overline{D_1^2})\,(\overline{D_1}) + 2\,(\overline{D_1})^3\right)$$

$$\begin{aligned}\mathcal{C}_4 = \overline{D_4} + 3\left(\overline{D_2^2} - (\overline{D_2})^2\right) + 4\left(\overline{D_3 D_1} - (\overline{D_3})\,(\overline{D_1})\right) + \\ 6\left(\overline{D_2 D_1^2} - (\overline{D_2})\,(\overline{D_1^2})\right) - 12\left((\overline{D_2 D_1})\,(\overline{D_1}) - (\overline{D_2})\,(\overline{D_1})^2\right) + \\ \left(\overline{D_1^4} - 4\,(\overline{D_1^3})\,(\overline{D_1}) + 12\,(\overline{D_1^2})\,(\overline{D_1})^2 - 6\,(\overline{D_1})^4 - 3\,(\overline{D_1^2})^2\right)\end{aligned}$$

$\overline{D_m^p D_n^q} \rightarrow$ unbiased $(p+q)^{th}$ power of D_m and D_n, for integers $m, n, p, q \geq 0$

Cumulant or X basis

In **cumulant** or $\boldsymbol{X}$ basis, we define a new variable $X_N = \sum_{n=1}^{N} \frac{\mu^n}{n!} D_n$

$$P^{X,M}_{ub,N} = \frac{1}{VT^3} \ln \mathcal{Z}^{X,M}_{ub,N}, \quad \mathcal{Z}^{X,M}_{ub,N} = \left\langle e^{Y^M_N(X)} \right\rangle, \quad Y^M_N(X) = \sum_{n=1}^{\boldsymbol{M}} \frac{\mathcal{L}_n(X_N)}{n!} \tag{10}$$

$\boldsymbol{M}$ cumulants, highest order derivative $\rightarrow$ $\boldsymbol{N}$. For $M = 4$, we have

$$\begin{aligned}
\mathcal{L}_1(X_N) &= \left(\overline{X_N}\right) \\
\mathcal{L}_2(X_N) &= \left[\left(\overline{X^2_N}\right) - \left(\overline{X_N}\right)^2\right] \\
\mathcal{L}_3(X_N) &= \left[\left(\overline{X^3_N}\right) - 3\left(\overline{X^2_N}\right)\left(\overline{X_N}\right) + 2\left(\overline{X_N}\right)^3\right] \\
\mathcal{L}_4(X_N) &= \left[\left(\overline{X^4_N}\right) - 4\left(\overline{X^3_N}\right)\left(\overline{X_N}\right) + 12\left(\overline{X^2_N}\right)\left(\overline{X_N}\right)^2\right. \\
&\quad \left. - 6\left(\overline{X_N}\right)^4 - 3\left(\overline{X^2_N}\right)^2\right]
\end{aligned}$$

$\overline{X^m_N}$ $\rightarrow$ unbiased m^{th} power of X_N

Cumulant expansion

- Considering $W_N = \sum_{n=1}^{N} \frac{\hat{\mu}^n}{n!} \bar{D}_n$, a possible cumulant expansion of exponential resummed form of ΔP as in eqn.(4) gives

$$\frac{\Delta P^C_{N,M}}{T^4} = \frac{1}{VT^3} \ln \left\langle e^{W_N} \right\rangle = \frac{1}{VT^3} \sum_{n=1}^{M} \frac{\kappa_n^N}{n!} + \mathcal{O}(\kappa^N_{M+1}) \tag{11}$$

$\boldsymbol{\kappa_n^N} \rightarrow \boldsymbol{n^{th}}$ cumulant with **highest** derivative order $\boldsymbol{N}$,
$\boldsymbol{M} \rightarrow$ **total** no. of cumulants. (Work : $M = 4$ and $N = 2, 4$ for μ_I)

- The cumulants κ_n^N, $1 \leq n \leq 4$ are given as follows

$$\begin{aligned}
\kappa_1^N &= \langle W_N \rangle , \\
\kappa_2^N &= \langle W_N^2 \rangle - \langle W_N \rangle^2 , \\
\kappa_3^N &= \langle W_N^3 \rangle - 3 \langle W_N^2 \rangle \langle W_N \rangle + 2 \langle W_N \rangle^3 \\
\kappa_4^N &= \langle W_N^4 \rangle - 4 \langle W_N^3 \rangle \langle W_N \rangle + 12 \langle W_N^2 \rangle \langle W_N \rangle^2 - 6 \langle W_N \rangle^4 - 3 \langle W_N^2 \rangle^2
\end{aligned} \tag{12}$$

- When $\boldsymbol{W_N^n \Rightarrow U_n[W_N]}$, we have $\boldsymbol{\kappa_n^N \Rightarrow \kappa_n^{N,ub}}$ (unbiased cumulants)
- $U_n[W_N]$ is unbiased n^{th} power of W_N. Consequences ??

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\end{aligned} \qquad (14)$$

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