Staggered rooting and unphysical phases at finite baryon density

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Introduction

- Lattice QCD simulations at finite density μ_B are typically based on analytic continuation from imaginary μ_B or Taylor expansion from $\mu_B = 0$, which becomes more unreliable as real μ_B increases
- In our search of critical point, in order to go further in μ_B , we attempt to do simulations directly at real $\mu_B > 0$ without relying on analytic continuation
- This can be done by reweighting:
  - Reweighting from $\mu_B = 0$
  - Sign Reweighting
  - Phase Reweighting
- In our recent calculations at $\mu_B > 0$ based on staggered action, problematic behavior is observed and it is believed to be due to rooting
- The goal of this talk:
  Our investigation of such issue and possible resolutions

Introduction

- Goal: $N_f = 2+1$ QCD simulation at $\mu_B > 0$ and $T > 0$
- Grand canonical partition function:

$$Z = \mathrm{Tr}\left[e^{-(H_{\mathrm{QCD}} - \mu_u N_u - \mu_d N_d - \mu_s N_s)/T}\right]$$

$$p = \frac{T}{V}\,\ln\, Z \equiv \hat{p}\; T^4$$

- Observables of interest:
  - Light quark density $\hat{n}_L \equiv \frac{\partial \hat{p}}{\partial \hat{\mu}_q}$
  - Susceptibility $\chi^l_n = \frac{\partial^n \hat{p}}{\partial \hat{\mu}^n_q}$
- $\hat{p}$ and its derivatives can be expanded in Taylor series in $\hat{\mu}_q$
- Scenario considered in this talk:

$$\hat{\mu}_q\; T \equiv \mu_q \equiv \mu_u = \mu_d = \frac{1}{3}\mu_B,\; \mu_s = 0$$

- To illustrate the issue, we will contrast with the scenario at finite μ_I:

$$\hat{\mu}_q\; T \equiv \mu_q \equiv \mu_u = -\mu_d = \mu_I,\; \mu_s = 0$$

Reweighting

- Simulation is impossible/hard in target ("t") action $\Rightarrow$ reweight from simulated ("s") action:

$$\langle O \rangle_t = \frac{\int D\phi w_t(\phi) O(\phi)}{\int D\phi w_t(\phi)} = \frac{\int D\phi w_s(\phi) \frac{w_t(\phi)}{w_s(\phi)} O(\phi)}{\int D\phi w_s(\phi) \frac{w_t(\phi)}{w_s(\phi)}} = \frac{\left\langle \frac{w_t}{w_s} O \right\rangle_s}{\left\langle \frac{w_t}{w_s} \right\rangle_s},$$

$$\frac{Z_t}{Z_s} = \left\langle \frac{w_t}{w_s} \right\rangle_s,$$

$$Z_t = \int D\phi w_t(\phi),\ w_t(\phi) \in \mathbb{C},\ \ Z_s = \int D\phi w_s(\phi),\ w_s(\phi) > 0$$

- Problems getting exponentially hard as V increases:
  - Sign problem: $\frac{w_t}{w_s} \in \mathbb{C}$
  - Overlap problem: $\rho\left(\frac{w_t}{w_s}\right)$ has long tail

Reweighting schemes

- Three reweighting schemes are considered:
  - Reweighting from $\mu_B = 0$: $\frac{w_t}{w_s} = \frac{\det M(\mu_B)}{\det M(0)}$

$$w_t = e^{-S_g} \det M(\mu_B),\ w_s = e^{-S_g} \det M(0)$$

  - Reweighting from Phase Quenched(PQ): $\frac{w_t}{w_s} = e^{i\theta(\mu_B)}$

$$w_t = e^{-S_g} \mid \det\ M(\mu_B) \mid e^{i\theta(\mu_B)},\ w_s = e^{-S_g} \mid \det\ M(\mu_B) \mid$$

  - Reweighting from Sign Quenched(SQ): $\frac{w_t}{w_s} = \mathrm{sign}(\cos\theta(\mu_B))$

$$w_t = e^{-S_g}\ \mathrm{Re}\ \det\ M(\mu_B),\ w_s = e^{-S_g}\ |\mathrm{Re}\ \det\ M(\mu_B)\ |$$

- Phase Reweighting and Sign Reweighting avoid overlap problem
- Sign Reweighting has milder sign problem than Phase Reweighting

[de Forcrand et al, NPB Proc. 2003; S. Borsanyi et al, Phys. Rev. D 105, L051506,2022]

Staggered Rooting at $\mu_B > 0$

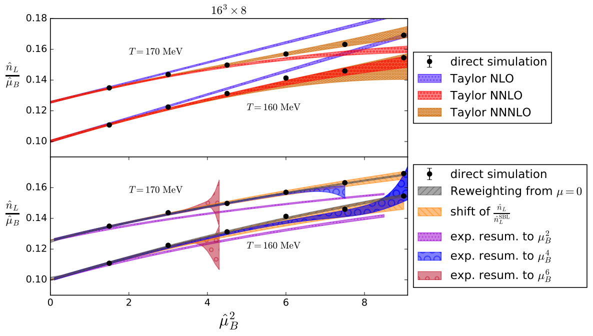
- Consider $N_f = 2+1$ at $\mu_q \equiv \mu_u = \mu_d = \mu_B/3$ and $\mu_s = 0$:

$$Z = \int dU \left[\det M_l(U, \mu_q)\right]^{\frac{1}{2}} \left[\det M_s(U)\right]^{\frac{1}{4}} e^{-S_g(U)}$$

- Definition of $(\det M_l)^{1/2}$ becomes ambiguous since now $\det M_l \in \mathbb{C}$
- Standard treatment: e.g.[Z. Fodor,S. Katz, JHEP 0203 (2002) 014; JHEP 0404 (2004) 050]
  Choose the root that continuously connects to the positive root at $\mu_B = 0$
- Question: Is it always the correct strategy to predict the right physics? How can we tell? [M. Golterman et al, PhysRevD 74(2006) 071501]

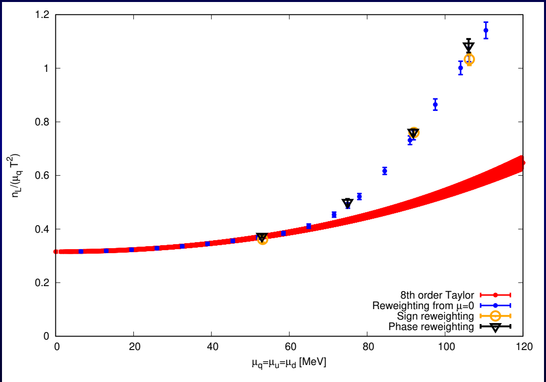
Staggered Rooting at $\mu_B > 0$

- In our reweighting simulations [S. Borsanyi et al, PhysRevD.107.L091503 (2022)], $\hat{n}_L$ at high T agrees with Taylor expansion



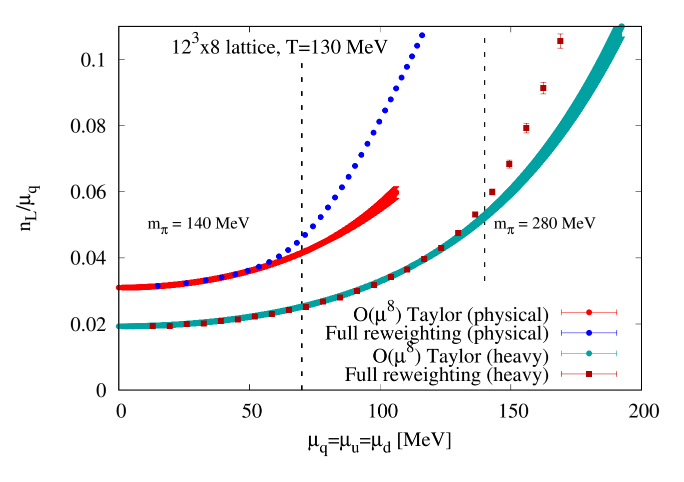
Staggered Rooting at $\mu_B > 0$

- Yet all three reweighted results deviate from it at low T :



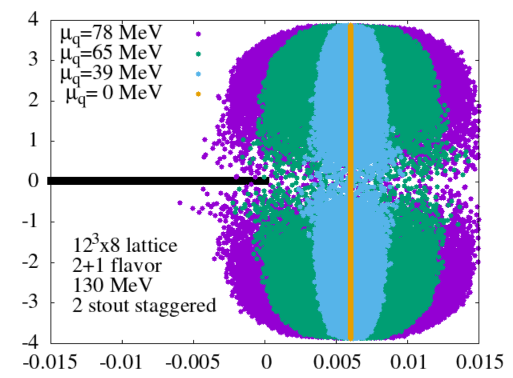
Staggered Rooting at $\mu_B > 0$

- This is observed at different pion masses, and the deviation becomes significant beyond $\mu_B \approx 3\, m_\pi/2$



Staggered Rooting at $\mu_B > 0$

- Rooting of $\det M_l$ introduces a branch cut in the spcetrum
- Analytic continuation from positive determination of the real square root $\Rightarrow$ The branch cut is along the negative real axis
- At $\hat{\mu} = 0$, the spectrum stays on the imaginary axis $\Rightarrow$ no ambiguity
- Turning on $\hat{\mu}$, the spectrum spreads out in the complex plane
- Such spread increases with $\hat{\mu}$
- Eventually a significant portion comes close to or crosses the branchcut $\Rightarrow$ creates ambiguity of which root is to be taken



Staggered Rooting at $\mu_B > 0$

- For $N_f = 4$, $\det M(\hat{\mu})$ can be expressed as follows in the temporal gauge: [Hasenfratz, Toussaint 1991]

$$\det M(\hat{\mu}) = e^{-3V\hat{\mu}} \prod_{i=1}^{6V} \left(\xi_i - e^{\hat{\mu}} \right)$$

where ξ_i are $6V = 6N_xN_yN_z$ eigenvalues of reduced matrix P that depend only on U and not μ

$$P = -\left(\prod_{i=0}^{N_t-1} P_i \right) L,\ P_i = \begin{pmatrix} B_i & 1 \\ 1 & 0 \end{pmatrix}\ B_i = \eta_4 (D^{(3)} + am)|_{t=i},\ L = \begin{pmatrix} U_4 & 0 \\ 0 & U_4 \end{pmatrix} |_{t=N_t-1}$$

- Rooting becomes:

$$[\det M_l(\hat{\mu})]^{1/2} = (\det M_l(0))^{1/2} \prod_{i=1}^{6V} \sqrt[\mathbb{C}]{\frac{\xi_i e^{\frac{\hat{\mu}}{2}} - e^{-\frac{\hat{\mu}}{2}}}{\xi_i - 1}}$$

- $[\det M(\hat{\mu})]^{1/2}$ therefore has a branchcut that creates ambiguity of which root is to be taken
- The portion of eigenvalues close to or crossing the branchcut increases with $\mu_B \Rightarrow$ Rooting becomes more ambiguous
- On the other hand, Taylor coefficients are computed at $\mu_B = 0$
- $\Rightarrow$ a non-analytic deviation between the two

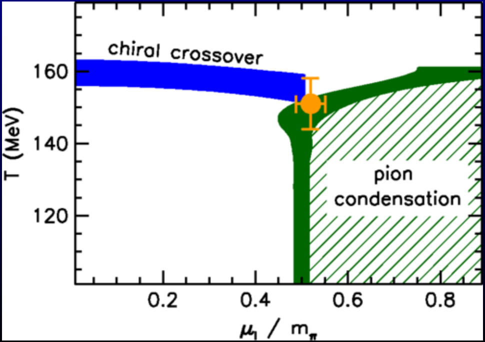
Comparison with physical phase transition

- In the case of $\mu_u = -\mu_d \equiv \mu, \mu_s = 0$, i.e. phase quenched (PQ), no complex rooting is involved

$$|\det M(\mu)|^2 = \det M(\mu_u = \mu) \det M(\mu_d = -\mu)$$

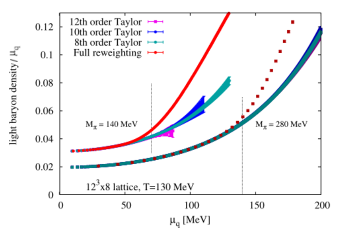
- it is equivalent to introducing an isospin chemical potential $\mu_I = \mu$
- It is well known that at $\mu_I \sim m_\pi/2$ at low T, there is a transition to pion-condensed phase

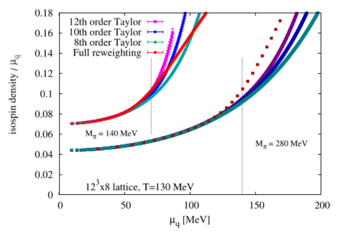
[Brandt, Endrödi, Schmalzbauer; PRD97, 054514 (2018);D.T. Son,M. Stephanov, Phys.Rev.Lett. 86 (2001) 592-595]



Comparison with physical phase transition

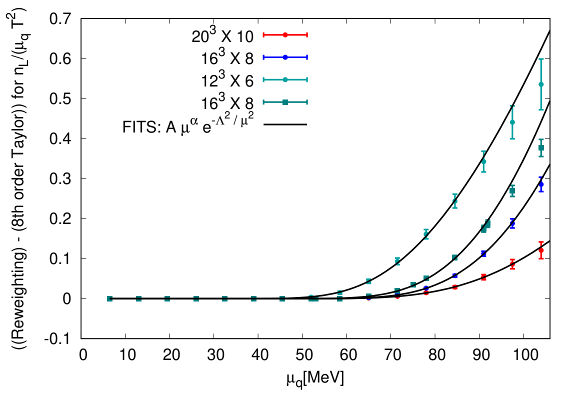
- If one probes physics at finite $\mu_I = \mu$ with $\mu_q = 0$ ensemble, a physical phase transition is observed at $\mu_I \approx m_\pi/2$ in both reweighted measurement and Taylor extrapolations
- If instead, one probes $\mu_q = \frac{1}{3}\mu_B = \mu$ with the same $\mu_q = 0$ ensemble, the reweighted measurements deviate from the Taylor extrapolations





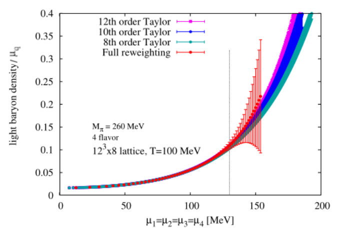
- $\Rightarrow$ The observed rise in the density with rooting is due to a singularity different from what is expected for a thermodynamic transition

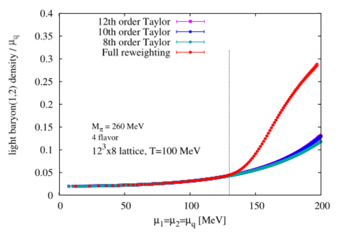
More evidence



- Such effect decreases with lattice spacing:
  - The effect is reduced by replacing stout-smearing with hex-smearing
  - also decreases as lattice spacing shrinks

More evidence





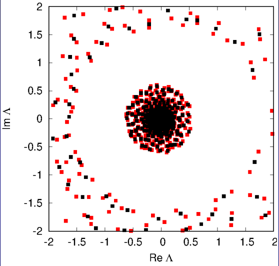
- Test this on $N_f = 4$:
  - It is not observed if not rooted (μ_q turned on for all four quarks)
  - It is observed if rooted (μ_q turned on for only two quarks)
  - Hints further that rooting is the culprit
- Is it better to simulate $N_f = 4$ then?
  - Sign problem is much worse $\ln\langle e^{i\theta}\rangle \propto \left(\frac{N_f \mu}{T}\right)^2 (LT)^3$
  - Less relevant to phenomenology

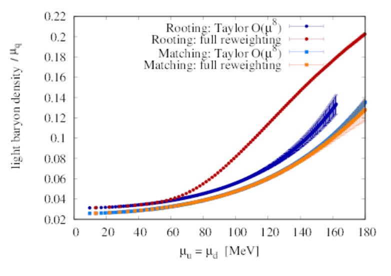
Conclusion

- In our simulations using rooted staggered actions at real $\mu_B > 0$, it is observed that at low T, the reweighted result deviates from Taylor extrapolations in the form of a sharp increase in light quark density beyond $\mu_B \approx 3m_\pi/2$
- Based on our investigation, such deviation decreases with spacings. It is likely that this behavior is a consequence of rooting and unphysical
- It is possible to remove the non-pertubative ambiguity by changing the definition of the finite μ determinant with geometric matching [M. Giordano et al, PhysRevD.101.074511(2020)], but this is a mixed action setup that non-locally modifies the determinant ⇒ further investigations needed
- The feasibility of using a minimally doubled action, Karsten-Wilczek action, is being investigated.
  More details will be discussed in Talks of R. Vig (Tue 16:20) and D. Godzieba (Tue 16:40). [Related: Talk by J. Weber (Wed 09:20)]

Geometric matching [Giordano, Kapas, Katz, Nogradi, Pasztor; PRD 2020]

- Replace neighboring eigenvalue doublets of ξ with geometric means (i.e. root before turning on μ)





- Feasible if one obtains all eigenvalues and taste breaking is not too severe(doublets recognizable)
- Non-perturbative terms at $\mu = 0$ zero are forbidden (no non-perturbative ambiguity), but different pairing algorithms (at finite spacing) will lead to different Taylor coefficients (a perturbative ambiguity)
- Redefined determinant no longer represents the target action $\Rightarrow$ turned into mixed action simulation

Finite volume effects?

- It is observed in different volumes