

New approach to lattice QCD at finite density: reweighting without an overlap problem

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Approaches to finite baryon density lattice QCD usually suffer from uncontrolled systematic uncertainties in addition to the well-known sign problem. We test a method - sign reweighting - that works directly at finite chemical potential and is yet free from any such uncontrolled systematics: with this approach the only problem is the sign problem itself. In practice the approach involves the generation of configurations with the positive fermionic weights given by the absolute value of the real part of the quark determinant, and a reweighting by a sign. There are only two sectors, +1 and -1 and as long as the average $\langle \pm \rangle \neq 0$ (with respect to the positive weight) this discrete reweighting has no overlap problem - unlike reweighting from $\mu = 0$ - and the results are reliable. We also present results based on this algorithm on the phase diagram of lattice QCD with two different actions: as a first test, we apply the method to calculate the position of the critical endpoint with unimproved staggered fermions at $N_\tau = 4$; as a second application, we study the phase diagram with 2stout improved staggered fermions at $N_\tau = 6$. This second one is already a reasonably fine lattice - relevant for phenomenology. We demonstrate that the method penetrates the region of the phase diagram where the Taylor and imaginary chemical potential methods lose predictive power.

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1. Introduction

One of the most important unsolved problems in QCD is the determination of the phase diagram of strongly interacting matter in the temperature-baryochemical potential plane. The most well-established method for first-principles studies of QCD is the lattice. Finite chemical potential lattice calculations are, however, hampered by the notorious sign- or complex-action problem. A number of approaches have been proposed to side-step this problem, such as reweighting [1–9], Taylor expansion around zero chemical potential [10–15], analytic continuation from purely imaginary chemical potentials [16–25], or the complex Langevin approach [26–28]. Unfortunately, all of these methods introduce extra problems, which are different from the sign problem itself, such as the analytic continuation problem of the Taylor and imaginary chemical potential methods, the overlap problem of reweighting and the Taylor method, or the convergence issues of complex Langevin. Often these problems are just as prohibiting as the original sign problem. It is therefore of value to have an alternative method, which does not have any of the extra problems of the existing methods: a method where the only problem is the sign problem itself.

Although manifesting as different, the analytic continuation problem of the Taylor and imaginary chemical potential methods and the overlap problem of the reweighting and Taylor methods have the same physical origin: an inability to directly sample the gauge configurations most relevant to finite chemical potential, thus requiring some kind of extrapolation in both cases. One would then like to perform simulations in a theory from which reconstruction of the desired theory is the least affected by such systematic effects, by (1) keeping as close as possible to the most relevant configurations, thus minimizing the overlap problem, and by (2) making the complex-action problem, or sign problem, due to cancellations among contributions, as mild as possible. We show here that such an approach - sign reweighting - has already become feasible on phenomenologically relevant lattices. This conference contribution is mainly based on Refs. [8, 9]

2. Reweighting and the overlap problem

A generic reweighting method reconstructs expectation values in a desired target theory, with microscopic variables U , path-integral weights $w_t(U)$, and partition function $Z_t = \int \mathcal{D}U w_t(U)$, using simulations in a theory with real and positive path-integral weights $w_s(U)$ and partition function $Z_s = \int \mathcal{D}U w_s(U)$, via the formula:

$$\langle O \rangle_t = \frac{\left\langle \frac{w_t}{w_s} O \right\rangle_s}{\left\langle \frac{w_t}{w_s} \right\rangle_s} \quad (1)$$

where $\langle \dots \rangle_t$ and $\langle \dots \rangle_s$ means expectation value in the target and the simulated theories respectively. When the target theory is lattice QCD at finite chemical potential, the target weights $w_t(U)$ have wildly fluctuating phases: this is the infamous sign problem. In addition to this problem, generic reweighting methods also suffer from an overlap problem: the probability distribution of the reweighting factor w_t/w_s has generally a long tail, which cannot be sampled efficiently in standard Monte Carlo simulations. The overlap problem is present even in cases when one tries to reweight to a theory without a sign problem, such as reweighting to a different bare gauge coupling. However,

even in the case of reweighting from zero to finite baryochemical potential, it is actually the overlap problem, rather than the sign problem, that constitutes the immediate bottleneck in QCD when one tries to extend reweighting results to finer lattices, even in the case of the multiparameter reweighting method [3], as was recently demonstrated by the study of the histogram of the reweighting factors w_t/w_s in Ref. [7].

A way to address the overlap problem is to reweight from a theory where the reweighting factors w_t/w_s takes values in a compact space. In such a case, their distribution does not have tails by construction, and so that the ratio $\frac{Z_t}{Z_s} = \left\langle \frac{w_t}{w_s} \right\rangle_s$ can be calculated without encountering any heavy-tailed distributions. The most obvious choice for the theory to reweight from is the phase quenched (PQ) theory, defined by

$$w_{PQ} = |\det M_{ud}(\mu)^{\frac{1}{2}}| |\det M_s(0)^{\frac{1}{4}}| e^{-S_g}, \quad (2)$$

where μ is the chemical potential of the light quarks, and for simplicity we take the strange quark chemical potential to be zero. In this case the reweighting factors are pure phases $e^{i\theta}$, where $\theta = \text{Arg}(\det M_{ud}(\mu)^{1/2})$. Another choice, which - as we will show - has a weaker sign problem is to reweight from the sign quenched (SQ) ensemble [8, 29, 30], defined by

$$w_{SQ} = |\text{Re} \det M_{ud}(\mu)^{\frac{1}{2}}| |\det M_s(0)^{\frac{1}{4}}| e^{-S_g}, \quad (3)$$

where reweighting involves only a sign factor:

$$\varepsilon = \text{sign} \cos \text{Arg} \det M_{ud}(\mu)^{\frac{1}{2}}. \quad (4)$$

We note that this amounts to the substitution of the determinant with its real part in the path integral, which is not permitted in arbitrary expectation values, but is completely valid for (1) observables that satisfy $O(U) = O(U^*)$ or (2) observables which can be defined as real derivatives of the partition function with respect to a real parameter, such as the gauge coupling, the quark mass or the chemical potential. While this set of observables is not exhaustive, it is enough to study bulk thermodynamics, which is the main target of our work.

3. Lattice simulations

As a first test of the method, in Ref. [8] we used unimproved staggered fermions on lattices of size $6^3 \times 4$, $8^3 \times 4$, $10^3 \times 4$ and $12^3 \times 4$ to estimate the position of the critical endpoint on these coarse lattices. For each lattice size and each chemical potential in the baryochemical potential range $0 \leq \hat{\mu}_B = \mu_B/T \leq 2.4$, we simulated one single value of the bare gauge coupling β , chosen to be close to the transition temperature at the given μ_B .

To move in the direction of the continuum limit, in Ref. [9] we used a tree level Symanzik improved gauge action with two steps of stout smearing with parameter $\rho = 0.15$ on $16^3 \times 6$ lattices [31]. We performed a scan in chemical potential at fixed $T = 140$ MeV, and a scan in temperature at fixed $\hat{\mu}_B = 1.5$.

In both cases, simulations were performed by modifying the RHMC algorithm at $\mu_B = 0$ by including an extra accept/reject step that takes into account the factor $\frac{|\text{Re} \det M_{ud}(\mu)^{\frac{1}{2}}|}{\det M_{ud}(0)^{\frac{1}{2}}}$. The determinant was calculated with the reduced matrix formalism [1] and dense linear algebra, with no stochastic estimators involved.

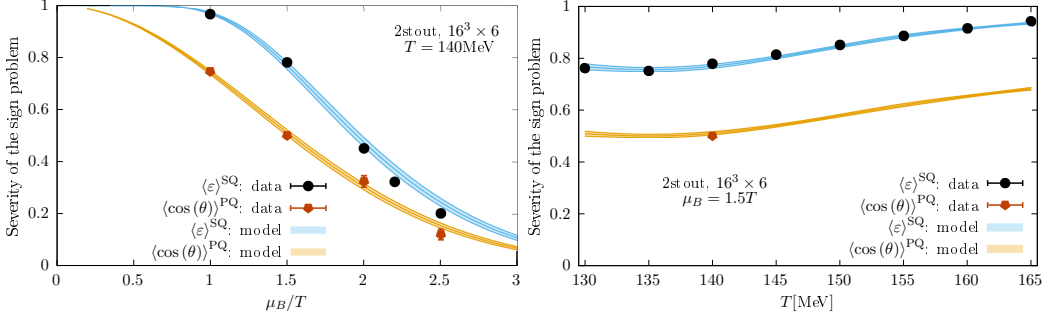


Figure 1: The strength of the sign problem on 2stout improved $16^3 \times 6$ staggered lattices as a function of μ_B/T at $T = 140 \text{ MeV}$ (left) and as a function of T at $\mu_B/T = 1.5$. A value close to 1 shows a mild sign problem, while a small value indicates a severe sign problem. Data for sign reweighting (black) and phase reweighting (orange) are from simulations. Predictions of the Gaussian model (see text) are also shown.

4. Comparison with phase reweighting and the strength of the sign problem

In the PQ ensemble the severity of the sign problem is measured by the average phase factor $\langle e^{i\theta} \rangle_{T,\mu}^{\text{PQ}} = \langle \cos \theta \rangle_{T,\mu}^{\text{PQ}}$, while in the SQ ensemble it is measured by the average sign $\langle \varepsilon \rangle_{T,\mu}^{\text{SQ}} = \langle \cos \theta \rangle_{T,\mu}^{\text{PQ}} / \langle |\cos \theta| \rangle_{T,\mu}^{\text{PQ}}$. Clearly, $\langle \cos \theta \rangle_{T,\mu}^{\text{PQ}} \leq \langle \varepsilon \rangle_{T,\mu}^{\text{SQ}}$, so the sign problem is generally weaker in the SQ case. To understand how much weaker it is, it is useful to introduce some small chemical potential approximations for the strength of the sign problem in both cases. The probability distribution of the phases $\theta = \arg \det M$ in the phase quenched theory, $P_{\text{PQ}}(\theta)$, controls the strength of the sign problem in both ensembles. A simple estimate can then be obtained with the following two steps: (i) in a leading order cumulant expansion, $P_{\text{PQ}}(\theta)$ is assumed to be a wrapped Gaussian distribution; (ii) the chemical potential dependence of its width is approximated by the leading order term in its Taylor expansion [10],

$$\sigma(\mu)^2 \approx \langle \theta^2 \rangle_{\text{LO}} = -\frac{4}{9} \chi_{11}^{ud} (LT)^3 \hat{\mu}_B^2, \quad (5)$$

where $\chi_{11}^{ud} = \frac{1}{T^2} \frac{\partial^2 p}{\partial \mu_u \partial \mu_d} |_{\mu_u = \mu_d = 0}$ is the disconnected part of the light quark susceptibility, obtained in $\mu = 0$ simulations. In this approximation the strength of the sign problem can be calculated analytically in both cases, with $\langle \cos \theta \rangle_{T,\mu}^{\text{PQ}} \approx e^{-\frac{\sigma^2(\mu)}{2}}$ in the phase quenched case, while in the sign quenched case the expression for $\langle \varepsilon \rangle_{T,\mu}^{\text{SQ}}$ is more involved. (See the Appendix of Ref. [9].) It is however worth noting the different asymptotics of the two cases. The small- μ (i.e., small- σ) asymptotics are notably very different, with $\langle \cos \theta \rangle_{T,\mu}^{\text{PQ}} \sim 1 - \frac{\sigma^2(\mu)}{2}$ analytic in $\hat{\mu}_B$, while in the sign quenched case $\langle \varepsilon \rangle_{T,\mu}^{\text{SQ}}$ is not analytic,

$$\langle \varepsilon \rangle_{T,\mu}^{\text{SQ}} \underset{\hat{\mu}_B \rightarrow 0}{\sim} 1 - \left(\frac{4}{\pi} \right)^{\frac{5}{2}} \left(\frac{\sigma^2(\mu)}{2} \right)^{\frac{3}{2}} e^{-\frac{\pi^2}{8\sigma^2(\mu)}}, \quad (6)$$

approaching 1 faster than any polynomial: therefore we expect the sign problem of the phase quenched ensemble to get worse faster at small μ_B as compared to the sign quenched case. The large- μ or large volume asymptotics are on the other hand quite similar: in the large- σ limit $P_{\text{PQ}}(\theta)$ tends to the uniform distribution, and so one arrives at $\frac{\langle \varepsilon \rangle_{T,\mu}^{\text{SQ}}}{\langle \cos \theta \rangle_{T,\mu}^{\text{PQ}}} \underset{\hat{\mu}_B \text{ or } V \rightarrow \infty}{\sim} \left(\int_{-\pi}^{\pi} d\theta |\cos \theta| \right)^{-1} = \frac{\pi}{2}$,

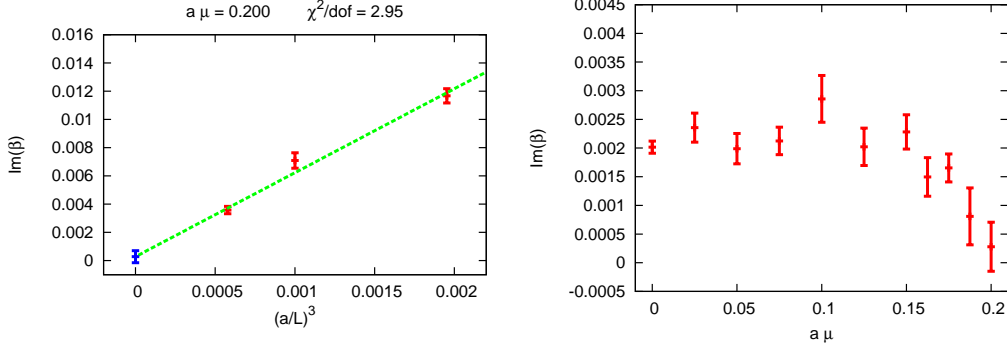


Figure 2: Finite volume scaling of the imaginary part of the leading Fisher zero at $\mu_B/T = 2.4$ (left) and the infinite volume extrapolated value of the imaginary part of the leading Fisher zero as a function of the chemical potential (right) for the unimproved staggered action at $N_\tau = 4$.

which asymptotically translates to a factor of $(\frac{\pi}{2})^2 \approx 2.5$ less statistics needed for a sign quenched simulation as compared to a phase quenched simulation.

The simple considerations made above are confirmed by actual simulation data to a decent degree, as can be seen in Fig. 1: our simple model predicts the strength of the sign problem both as a function of μ_B at a fixed temperature (left) and as a function of temperature at a fixed μ_B/T (right). This is of great practical importance, as it makes the planning of future simulation projects with reweighting relatively straightforward.

5. Physics observables

5.1 Unimproved action at $N_\tau = 4$

The main goal of our first numerical study in Ref. [8] was to confirm or falsify the critical endpoint prediction of Ref. [3] for the unimproved staggered discretization at temporal extent $N_\tau = 4$, with a method that does not suffer from an overlap problem in the reweighting factors. To be as close to Ref. [3] as possible, we therefore use the same physical observable and computed the zeros of the partition function in the bare gauge coupling β , the so-called Fisher zeros. This amounts to measuring the observables $O_\beta(U) = e^{-\frac{\beta - \beta_s}{\beta_s} S_g(U)}$, where $S_g(U)$ is the gauge action and β_s is the simulated bare coupling. Since $O_\beta(U^*) = O_\beta(U)$, sign reweighting can be applied to this observable. The partition function has several zeros as a function of complex β . We computed the one closest to the real axis, which in every run happens to coincide with the one closest to the simulation point in the β as well. This zero will be called the leading Fisher zero. The finite volume scaling and the infinite volume extrapolated leading zero position can be seen in Fig. 2. As can be seen in that Figure, the leading Fisher zero extrapolates to a point on the real line at around $\mu_B/T = 2.4$, in agreement with the result of Ref. [3].

5.2 Two-stout improved action at $N_\tau = 6$

We now proceed to display physics results for the light quark condensate and density from simulations with the 2stout improved staggered action at $N_\tau = 6$. The light-quark chiral condensate

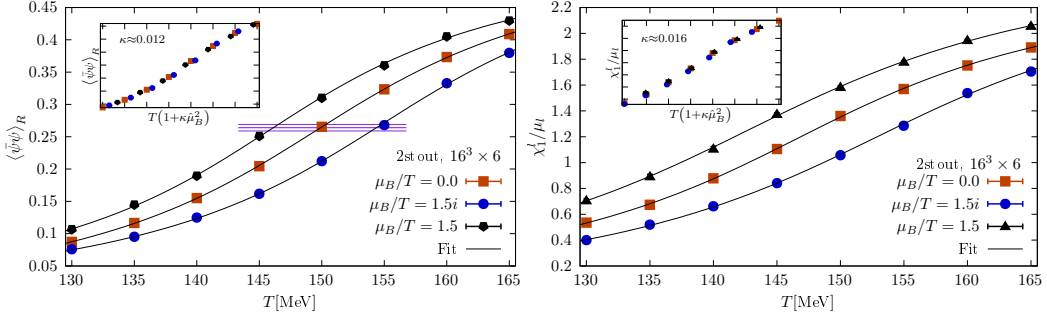


Figure 3: The renormalized chiral condensate (left) and the light quark number-to-light quark chemical potential ratio (right) as a function of T at fixed $\mu_B/T = 1.5, 0$ and $1.5i$ on 2stout improved lattices at $N_\tau = 6$. The insets show a rescaling of the temperature axis, which approximately collapses the curves onto each other.

was obtained via the formula

$$\langle \bar{\psi}\psi \rangle_{T,\mu} = \frac{1}{Z(T,\mu)} \frac{\partial Z(T,\mu)}{\partial m_{ud}} = \frac{T}{V} \frac{1}{\langle \varepsilon \rangle_{T,\mu}^{\text{SQ}}} \left\langle \varepsilon \frac{\partial}{\partial m_{ud}} \ln \left| \text{Re det } M_{ud}^{\frac{1}{2}} \right| \right\rangle_{T,\mu}^{\text{SQ}}, \quad (7)$$

with the determinant $\det M = \det M(U, m_{ud}, m_s, \mu)$ calculated in the reduced matrix formalism at different light-quark masses and fed into a symmetric difference, $\frac{df(m)}{dm} \approx \frac{f(m+\Delta m) - f(m-\Delta m)}{2\Delta m}$. The step Δm small enough to make the systematic error from the finite difference negligible compared to the statistical error. The renormalized condensate was obtained with the prescription

$$\langle \bar{\psi}\psi \rangle_R(T, \mu) = -\frac{m_{ud}}{f_\pi^4} \left[\langle \bar{\psi}\psi \rangle_{T,\mu} - \langle \bar{\psi}\psi \rangle_{0,0} \right]. \quad (8)$$

We also calculated the light quark density

$$\chi_1^l \equiv \frac{\partial (p/T^4)}{\partial (\mu/T)} = \frac{1}{VT^3} \frac{1}{Z(T,\mu)} \frac{\partial Z(T,\mu)}{\partial \hat{\mu}} = \frac{1}{VT^3 \langle \varepsilon \rangle_{T,\mu}^{\text{SQ}}} \left\langle \varepsilon \frac{\partial}{\partial \hat{\mu}} \ln \left| \text{Re det } M_{ud}^{\frac{1}{2}} \right| \right\rangle_{T,\mu}^{\text{SQ}}, \quad (9)$$

evaluating the derivative analytically using the reduced matrix formalism. This quantity does not have to be renormalized.

Our results for the temperature scan at $\mu_B/T = 1.5$ are shown in Fig. 3. We also show the corresponding curves at zero and the imaginary value of $\mu_B/T = 1.5i$ for comparison. We also show a rescaling of the temperature axis, collapsing the curves into each other, and demonstrating that at least up to $\mu_B/T = 1.5$ the chiral crossover does not get narrower. Our results for the chemical potential scan at a fixed temperature of $T = 140$ MeV are shown in Fig. 4. We have performed simulations at $\hat{\mu}_B = 1, 1.5, 2, 2.2, 2.5, 2.7$. The point at $\hat{\mu}_B = 2.2$ corresponds roughly to the chiral transition, as at this point the chiral condensate is close to its value at the $\mu_B = 0$ crossover. The sign-quenched results are compared with the results of analytic continuation from imaginary chemical potentials. To demonstrate the magnitude of the systematic errors of such an extrapolation we considered two fits. (i) As the simplest ansatz, we fitted the data with a cubic polynomial in $\hat{\mu}_B^2$ in the range $\hat{\mu}_B^2 \in [-10, 0]$. (ii) As an alternative, we also used suitable ansätze for $\langle \bar{\psi}\psi \rangle_R$ and $\chi_1^l/\hat{\mu}_l$ based on the fugacity expansion $p/T^4 = \sum_n A_n \cosh(n\hat{\mu})$, fitting the data in

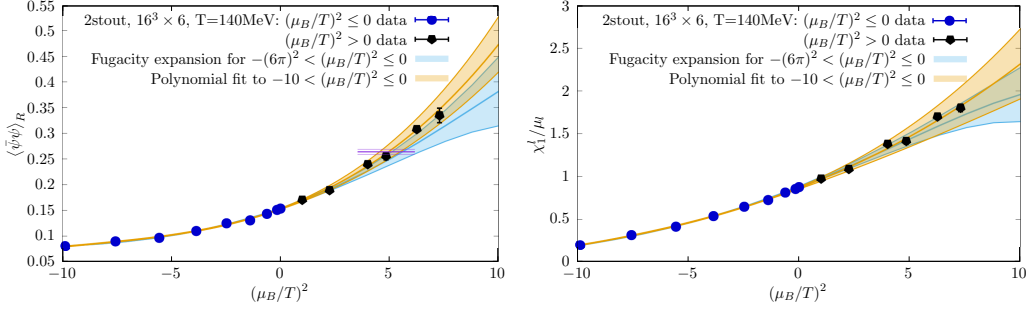


Figure 4: The renormalized chiral condensate (left) and the light quark number-to-light quark chemical potential ratio (right) as a function of $(\mu_B/T)^2$ at temperature $T = 140$ MeV with the 2stout improved staggered action at $N_\tau = 6$. Data from simulations at real μ_B (black) are compared with analytic continuation from simulations at imaginary μ_B (blue). In the left panel the value of the condensate at the crossover temperature at $\mu_B = 0$ is also shown by the horizontal line. The simulation data cross this line at $\mu_B/T \approx 2.2$.

the entire imaginary-potential range $\hat{\mu}_B^2 \in [-(6\pi)^2, 0]$ using respectively 7 and 6 fitting parameters. Fit results are also shown in Fig. 4; only statistical errors are displayed. While sign reweighting and analytic continuation give compatible results, in the upper half of the μ_B range the errors from sign reweighting are an order of magnitude smaller. In fact, sign reweighting can penetrate the region $\hat{\mu}_B > 2$ where the extrapolation of many quantities is not yet possible with standard methods [13, 22].

6. Summary

Sign reweighting has opened up a new window to study the bulk thermodynamics of strongly interacting matter from first principles. While the method is ultimately bottlenecked by the sign problem, in the region of its applicability it offers excellent reliability compared to the dominant methods of Taylor expansion and imaginary chemical potentials - which always provide results having a shadow of a doubt hanging over them due to the analytic continuation problem. We have demonstrated that the strength of the sign problem can be easily estimated with $\mu = 0$ simulations, making the method practical and the planning of simulation projects straightforward. We have also demonstrated that the method extends well into the regime where the established methods start to lose predictive power and covers the range of the RHIC BES.

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